EDGEWOOD
RESEARCH DEVELOPMENT & ENGINEERING CENTER
U.S. ARMY CHEMICAL AND BIOLOGICAL DEFENSE COMMAND

ERDEC-TR-112

THEORETICAL PREDICTION OF VIBRATIONAL CIRCULAR DICHROISM SPECTRA OF R-GLYCERALDEHYDE, R-ERYTHROSE, AND R-THREOSE

I. COMPUTATIONAL RESULTS

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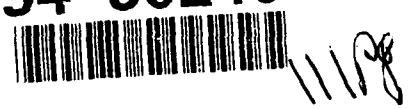

November 1993

Aberdeen Proving Ground, MD 21010-5423

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	1993 November	Final, 92 May - 92 Oct

4. TITLE AND SUBTITLE
Theoretical Prediction of Vibrational Circular Dichroism Spectra of R-Glyceraldehyde, R-Erythrose, and R-Threose
I. Computational Results

5. FUNDING NUMBERS
PR-1O162622A553C
PR-1O161102A71A
C-DAAL03-91-C-0034
D.O.-181

6. AUTHOR(S)
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DIR, ERDEC,* ATTN: SCBRD-RTE, APG, MD 21010-5423

8. PERFORMING ORGANIZATION REPORT NUMBER
ERDEC-TR-112

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
DIR, ARO, P.O. Box 12211, Research Triangle Park, NC 27709

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
TCN 92128

11. SUPPLEMENTARY NOTES
Task was performed under a Scientific Services Agreement issued by Battelle, Research Triangle Park Office, 200 Park Drive, P.O. Box 12297, Research Triangle Park, NC 27709
(Continued on page ii)

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*
A very important objective of the Detection Directorate at the U.S. Army Edgewood Research, Development and Engineering Center* is the remote detection of biological materials in the field. One line of thinking, currently being followed, is the recognition that sugars are distinguishing features of biological materials. Part I of this study reports on the theoretical prediction of the vibrational circular dichroism (VCD) of the 3 and 4 carbon sugars - R-glyceraldehyde, R-erythrose, and R-threose. The procedure involves optimization of geometries at the 3-21G HF and the 6-31G* HF levels and the subsequent determination of normal mode frequencies and rotational strengths to provide a nonscaled force constant result. To implement a scaling procedure, 8 small molecules containing 4-12 atoms were studied. Optimized geometries, frequencies and force constant matrices were determined based on calculations at the 3-21G HF, 3-21G MP2, 6-31G* HF, and 6-31G* MP2 levels of calculation. A set of scaling constants were determined by scaling 6-31G* HF calculated diagonal force constants to the 6-31G* MP2 level calculations. The scaling constant for each off-diagonal element of the force constant matrix was determined by using the geometric mean $Q_{ij} = (Q_i Q_j)^{1/2}$ of the diagonal scaling constants Q_i and Q_j. Couplings of various off-diagonal elements of the force constant matrix are reported. These scale factors were used to predict the VCD spectrum for the 3 sugars under study.

14. SUBJECT TERMS
Vibrational circular dichroism
Scaling of force constant matrix
R-glyceraldehyde
R-erythrose
R-threose

15. NUMBER OF PAGES
112

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

11. SUPPL[illegible]NTARY NOTES (Continued)

*When this study was conducted, ERDEC was known as the U.S. Army Chemical Research, Development and Engineering Center, and the ERDEC authors were assigned to the Research Directorate and U.S. Army Information Systems Command, respectively.

PREFACE

The work described in this report was authorized under Project No. 1O162622A553C, Reconnaissance, Detection, and Identification, Project No. 1O161102A71A, Research in CW/CB Defense, Contract No. DAAL03-91-C-0034, and Delivery Order No. 181. This work was started in May 1992 and completed in October 1992.

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Acknowledgments

This work was supported by the U.S. Army Edgewood Research, Development and Engineering Center (ERDEC)* (Dr. James O. Jensen) under the auspices of the U.S. Army Research Office Scientific Services Program administered by Battelle.

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THEORETICAL PREDICTION OF VIBRATIONAL CIRCULAR DICHROISM SPECTRA OF R-GLYCERALDEHYDE, R-ERYTHROSE, AND R-THREOSE

I. COMPUTATIONAL RESULTS

I.1 INTRODUCTION

One of the most important technologies in the master plan of the Reconnaissance, Detection and Identification (RDI) program at the Edgewood Research, Development and Engineering Center (ERDEC) is the remote detection, based on processes occurring in the infrared (IR), of hazardous biological materials in the field. At present ERDEC is a leader in the development of remote IR detectors. An experimental technique currently being developed under the leadership of A. H. Carrieri [1] at ERDEC is Mueller Matrix Spectroscopy [2,3]. The Phase Sensitive Detection Apparatus recently developed at ERDEC is the only infrared Mueller matrix spectrometer in the world. One feature obtained by such spectroscopy is the vibrational circular dichroism (VCD) spectrum of a molecular species [4-16]. This spectrum can be used as a unique fingerprint of a substance. Chiral molecules present in biological systems exhibit vibrational circular dichroism. Simulation of VCD spectra can serve two purposes:

1. Simulated spectra can go hand-in-hand with experiments. This interplay between experiment and theory will reinforce both areas of approach and will lead to improved means of accurate detection.
2. Theoretically predicted spectra can be helpful when direct experimentation is difficult or hazardous.

The present study is directed toward the theoretical prediction of the VCD spectra of the three sugars, R-glyceraldehyde, R-erythrose, and R-threose [17]. The method of calculation depends on Stephens' formulation of the rotational strength [5]; the following *ab initio* quantum chemical techniques were used: Gaussian 90, Gaussian 92, CADPAC version 4.2, and CADPAC version 5.0 [18-22]. These programs were operational on the STARDENT 3000 computers in the Berger Building (E3549) and the CONVEX computer at ERDEC. We performed *ab initio* quantum chemical calculations of the equilibrium geometries of the three sugar molecules [R-glyceraldehyde R-erythrose, R-threose]. At the equilibrium geometries we calculated the normal mode frequencies and rotational strengths at the Self-Consistent Field (SCF) level of theory using 3-21 G and 6-31G* basis sets. Since vibrational frequencies calculated at the SCF level of theory tend to be 10-15% higher than experimental values. A correction procedure was developed since the normal mode frequencies and the VCD rotational strengths would be error. The correction procedure that we considered was to obtain scaling constants for the contribution of various internal coordinates in the force constant matrix. This procedure involved the determination of the scaling constants for a set of 8 reference molecules. On the assumption of transferrability of these scaling constants from molecule-to-molecule the scaled force constant matrix for each of the 3 sugars of interest was determined. At this point the normal modes of vibration and the rotational strengths can then be determined from the scaled force constant matrix.

I.2 SCALING OF THE FORCE CONSTANT MATRIX

In order to implement a scaling procedure for the force constant matrix of a sugar a set of scaling factors for a set of 8 reference molecules, containing 4-12 atoms, were obtained. The reference set of molecules are

1. formaldehyde (CH_2O)
2. acetaldehyde (C_2H_4O)
3. methanol (CH_4O)
4. ethanol (C_2H_6O)
5. isopropanol (C_3H_8O)
6. dimethyl ether (C_2H_6O)
7. hydroxymethyl methyl ether ($C_2H_6O_2$)
8. ethylene glycol ($C_2H_6O_2$)

The scaling factors were determined in the following way. Optimized geometries, frequencies of vibration and force constant matrices were determined based on calculations at the 3-21G HF, 3-21G MP2, 6-31G* HF, and 6-31G* MP2 levels of calculation. In Tables 1a-8a the optimized geometries and frequencies are reported, in Tables 1b-8b the force constant matrices at the 6-31G* HF level of calculation are reported, and in Tables 1c-8c force constant matrices at the 6-31G* MP2 levlel of calculation are reported.

The diagonal scaling constants Q_i were determined by scaling the 6-31G* HF calculated force constants to the 6-31G* MP2 calculated force constants as

$$Q_i=F_{ii}(MP2)/F_{ii}(HF). \tag{1}$$

The off diagonal scaling constants Q_{ij} were determined by using the geometric mean of the diagonal constants involved

$$Q_{ij}=(Q_iQ_j)^{1/2}. \tag{2}$$

As a means of testing the goodness of the geometric mean fit we determined the matrix element C_{ij} as

$$C_{ij}=F_{ij}(MP2)/Q_{ij}F_{ij}(HF). \tag{3}$$

For values of F_{ij} less than 10^{-4}, C_{ij} is set to 1. As a result the goodness of the geometric mean fit is represented by the closeness of each C_{ij} to 1.

In Tables 1d-8d the set of Q_i 's and the set of C_{ij} 's are reported for each of the 8 molecules studied. Some of the C_{ij} 's that differ from 1 can be rationalized as due to possible coupling to another internal coordinate. However, in other cases the coupling is unexpected and may be an artifact of the method used. More time and study is required to investigate these couplings of different internal coordinates. Indeed, the original choice of the set of internal coordinates may be quite crucial in order to arrive at couplings which are quite small.

Using the results of Tables 1d-8d an average scaling factor for a given internal coordinate is determined. The results are reported in Table 9. Remarkably most internal coordinates give scaling factors in the neighborhood of 0.9 with the exception of a C=O stretch which gives a scaling of 0.772.

Next, we turn attention to the 3 sugars of interest in this project.

I.3 NONSCALED AND SCALED VCD SPECTRA FOR 3 SUGARS

We next consider optimization of the geometry of the 3 sugars under study. The geometries are optimized at the 3-21G and the 6-31G * HF levels. The results are reported in Tables 10-12. The optimized geometries for the 6-31G* calculations are shown in Figures 1-3. The VCD spectrum consists of a plot of the rotational strength R as a function of the the frequencies of vibration. The rotational strength R is obtained by

$$R = Im(\mu \cdot m) \qquad (4)$$

where μ is the electric dipole transition moment between the v=0 and the v=1 vibrational states, m is the magnetic dipole transition moment between the v=0 and the v=1 vibrational states and Im means to take the imaginary part of what follows. Calculated frequencies and rotational strengths based on the 3-21G HF level of calculation are reported in Tables 13-15. VCD spectra are shown in Figures 4-6 based on use of the harmonic oscillator approximation. The scaling parameters determined in Table 9 are used to scale the force constant matrix for each sugar based on the 6-31G* HF level of calculation. The resultant frequencies and rotational strengths for both unscaled and scaled 6-31G* HF calculations are shown in Tables 16-18. VCD spectra for the 6-31G* level of calculation are displayed in Fgures 7-9 based on use of the harmonic oscillator approximation. As is expected, frequencies of vibration are reduced by a factor of roughly 0.9. Rotational strengths of relatively large magnitude, after scaling, appear to retain their same sign and relatively large magnitude.

I.4 SUMMARY

This study represents continuing work toward the goal of generating theoretically predicted VCD spectra of sugars. The approach involves the use of Stephens' theoretical formulation of the rotational strength and the use of Gaussian calculations at the 3-21G and the 6-31G* levels. The level of calculation affects the frequencies and the rotational strength.

Originally, measurements of the VCD of several sugars were to be made at ERDEC using a recently acquired NICOLET FTIR instrument with a special engineered VCD attachment. Difficulty was encountered in reproducing the literature VCD spectrum of carvone with this instrument. The instrument is being inspected by NICOLET to determine the reason for the discrepancy. Because of the VCD instrument problem no comparison with experimental VCD spectra can be made at this time. Comparison awaits the resolution of the instrument problem by NICOLET. Once this is accomplished the experimental spectrum can be determined and the results of this study can be compared with the experimentally determined results.

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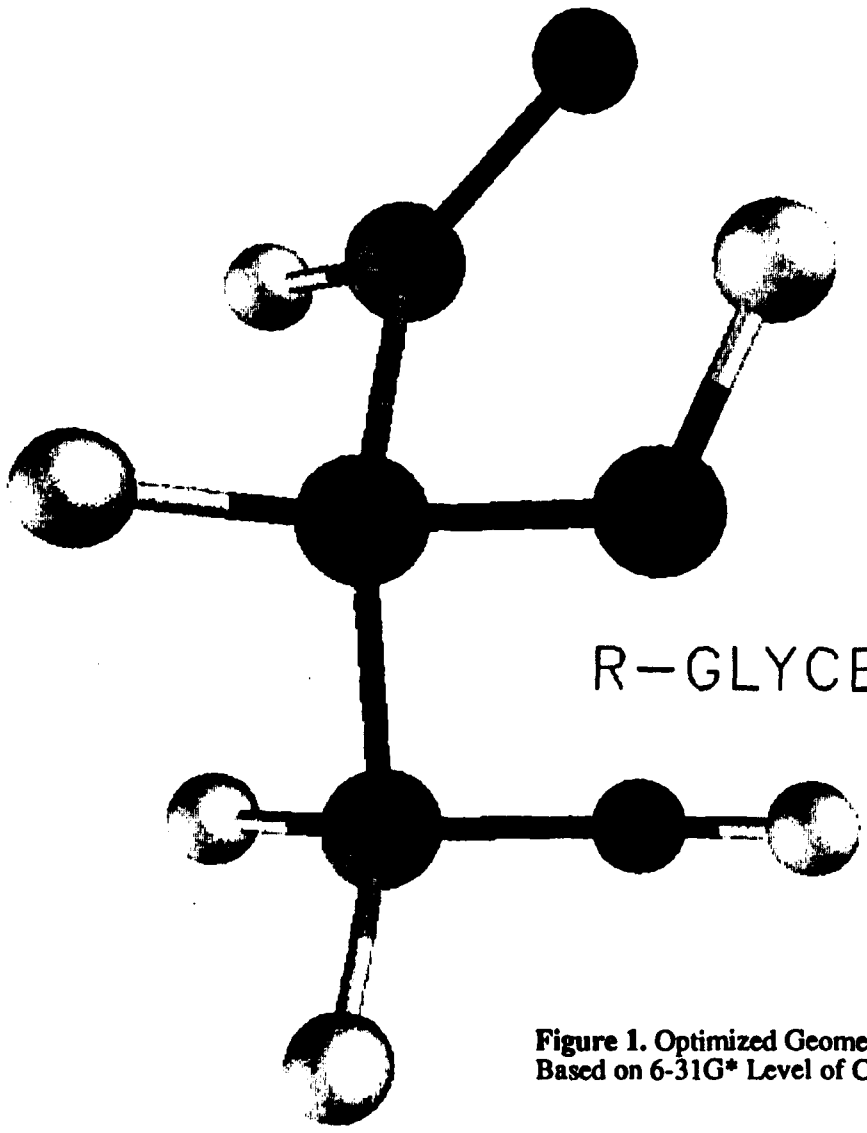


Figure 1. Optimized Geometry for R-Glyceraldehyde [CHO-HCOH-CH_2OH] Based on 6-31G* Level of Calculation.

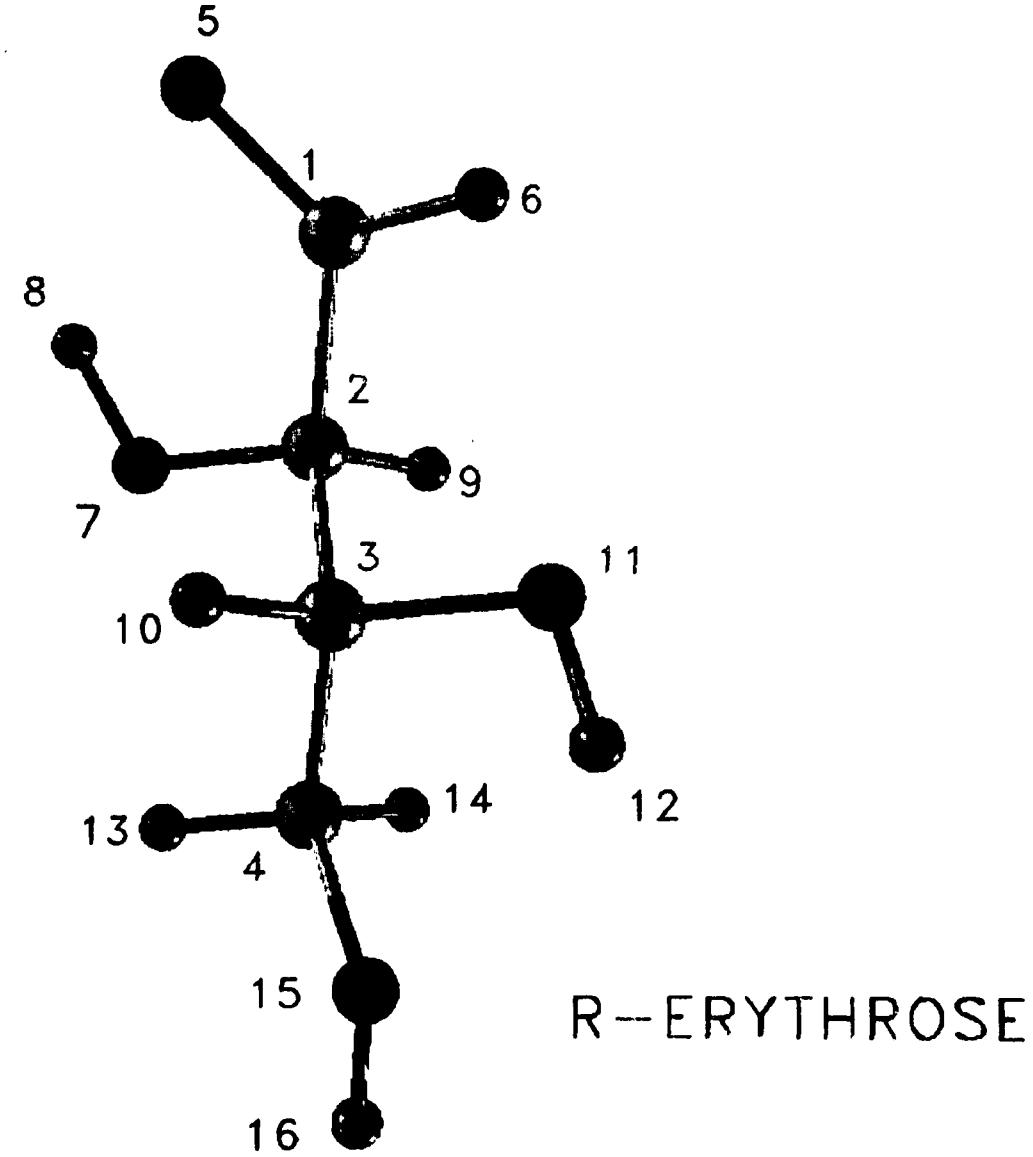


Figure 2. Optimized Geometry for R-Erythrose [CHO-HCOH-HCOH-CH_2OH] Based on 6-31G* Level of Calculation.

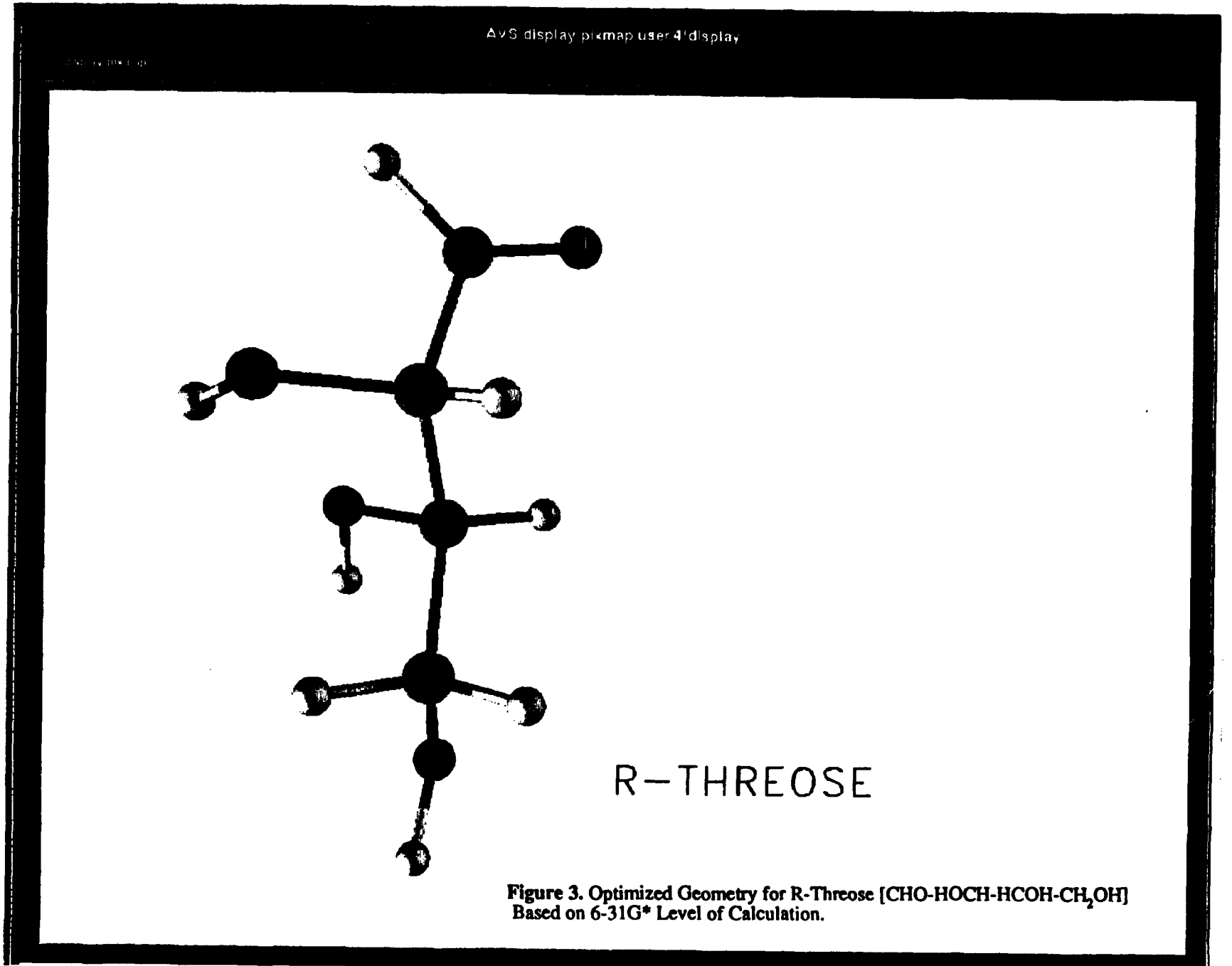


Figure 3. Optimized Geometry for R-Threose [CHO-HOCH-HCOH-CH_2OH] Based on 6-31G* Level of Calculation.

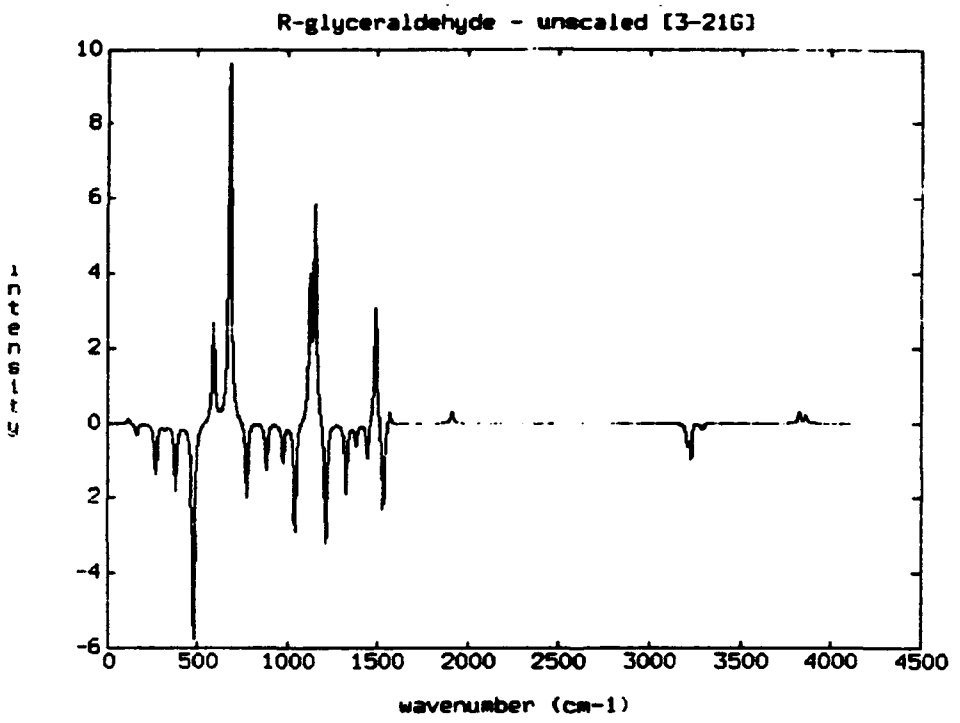


Figure 4. VCD Spectrum of R-Glyceraldehyde [CHO-HCOH-CH_2OH] Based on 3-21G Level of Calculation.

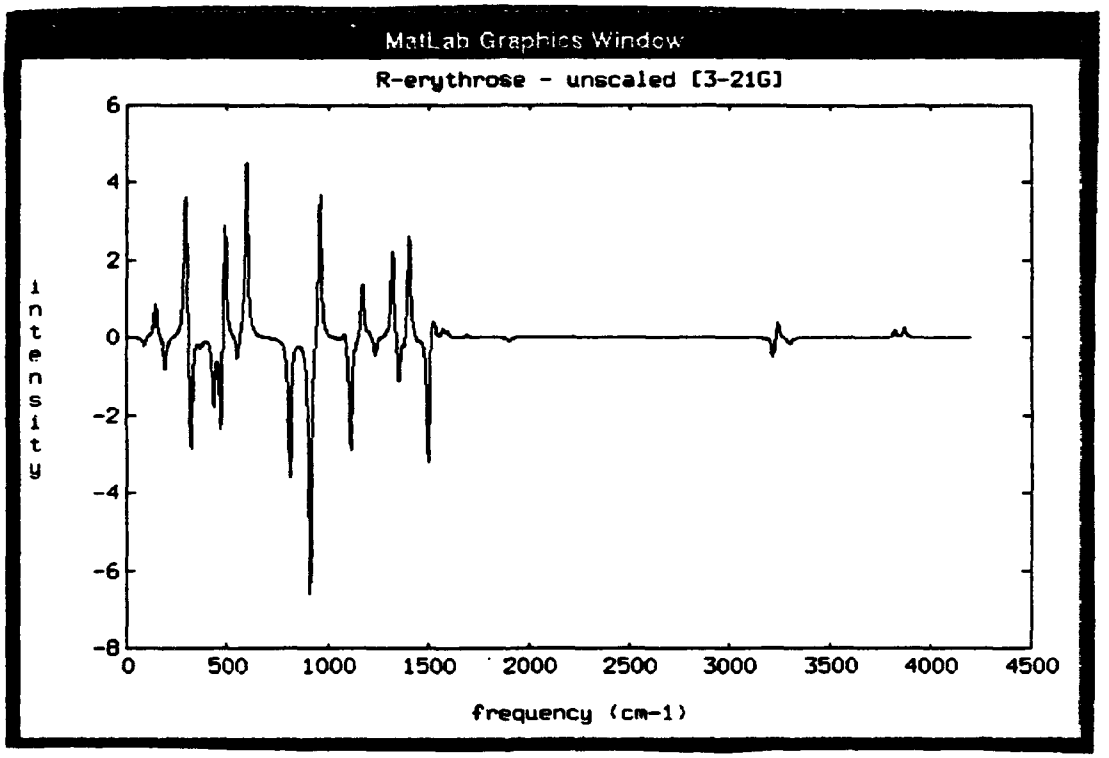


Figure 5. VCD Spectrum of R-Erythrose [CHO-HCOH-HCOH-CH_2OH] Based on 3-21G Level of Calculation.

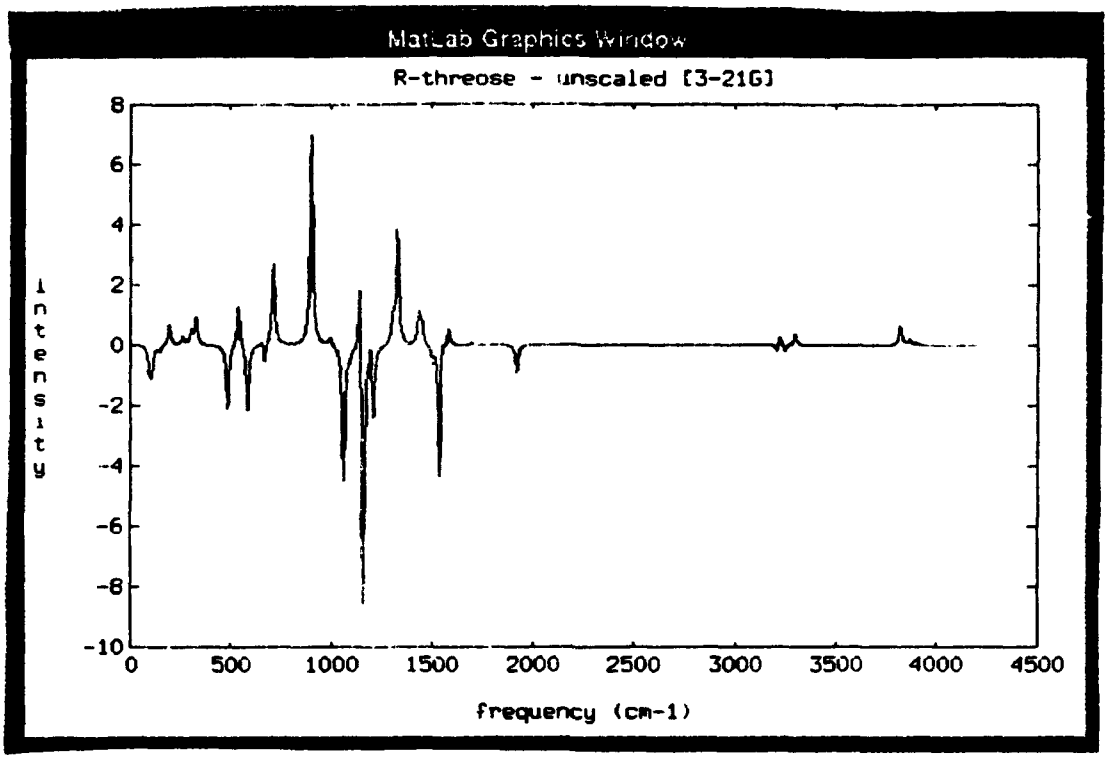
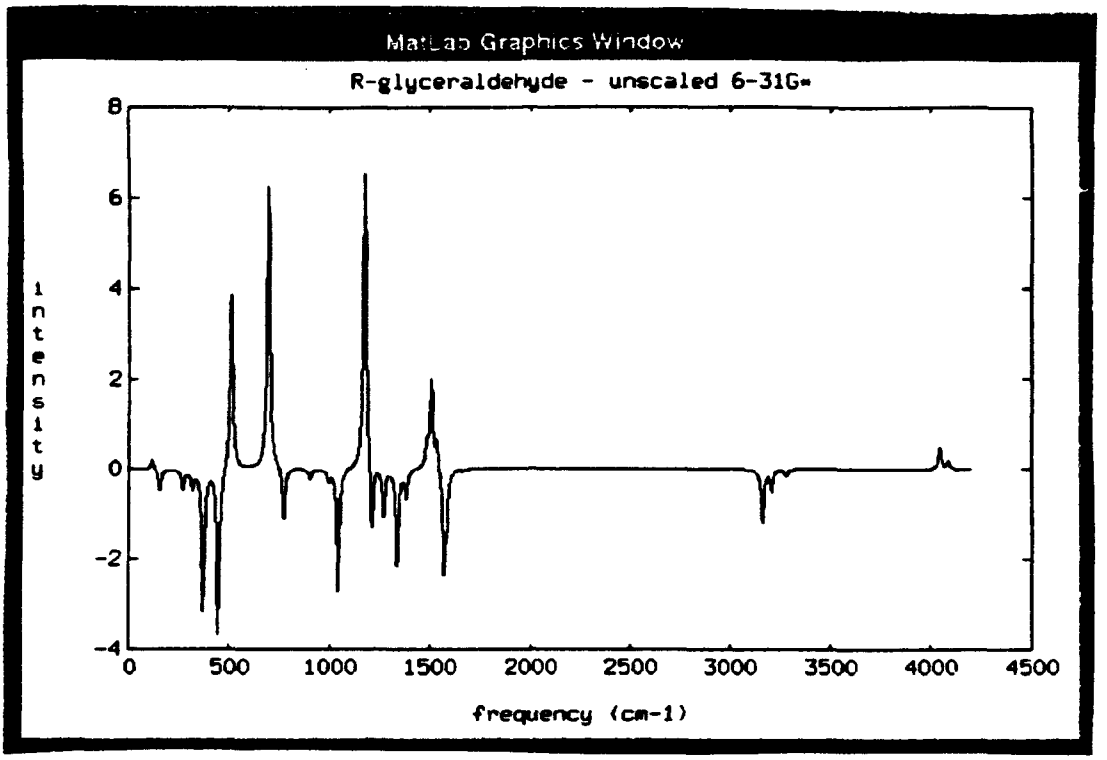


Figure 6. VCD Spectrum of R-Threose [CHO-HOCH-HCOH-CH_2OH] Based on 3-21G Level of Calculation.

(a)



(b)

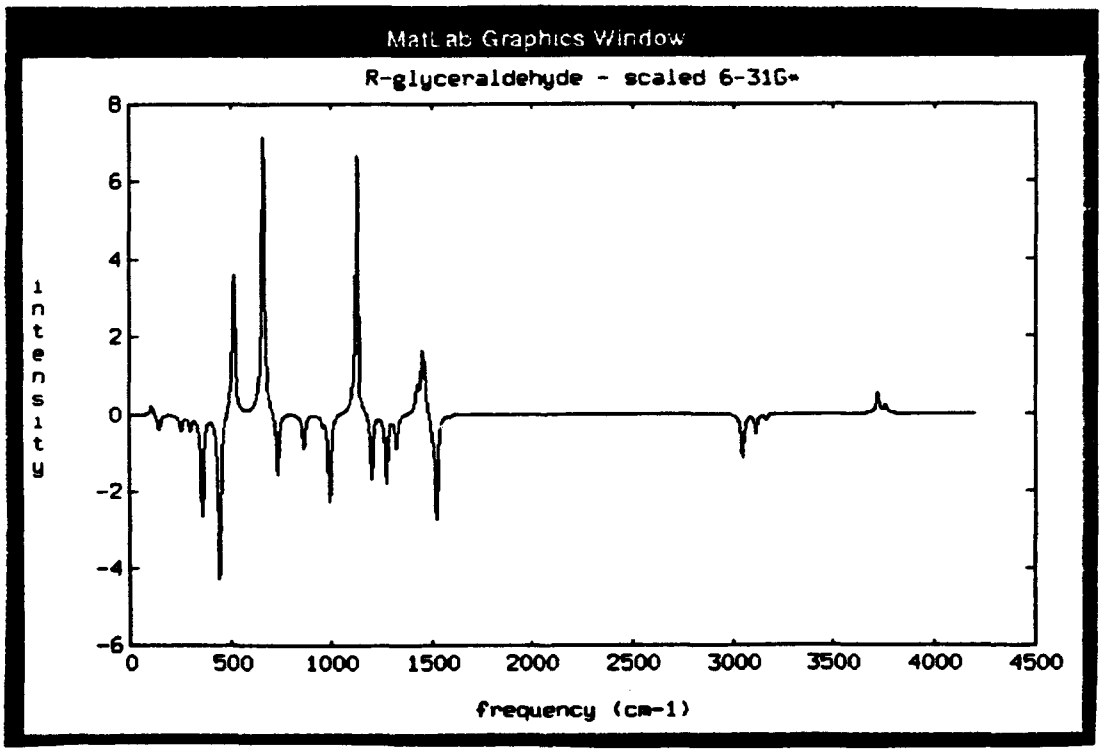
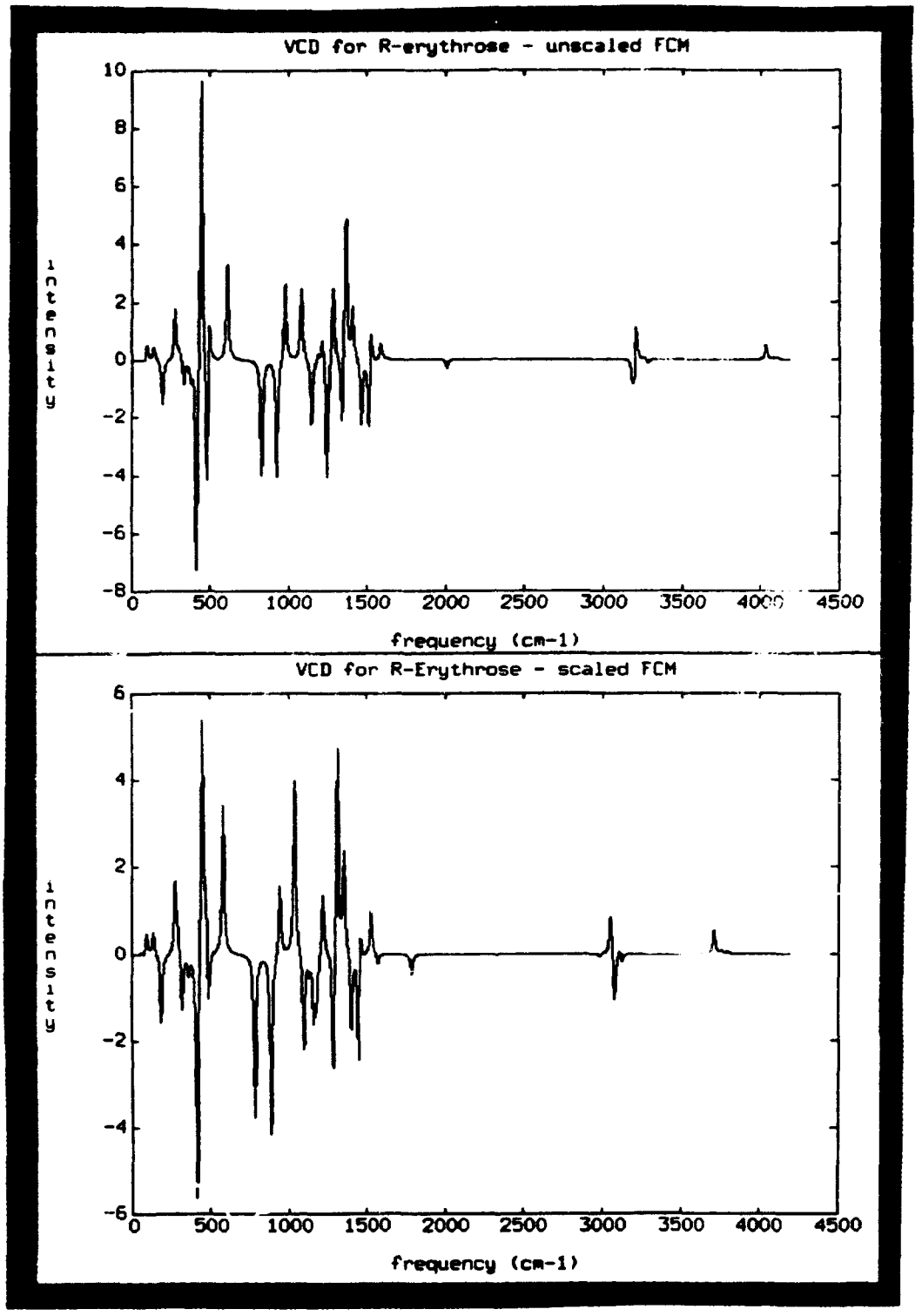


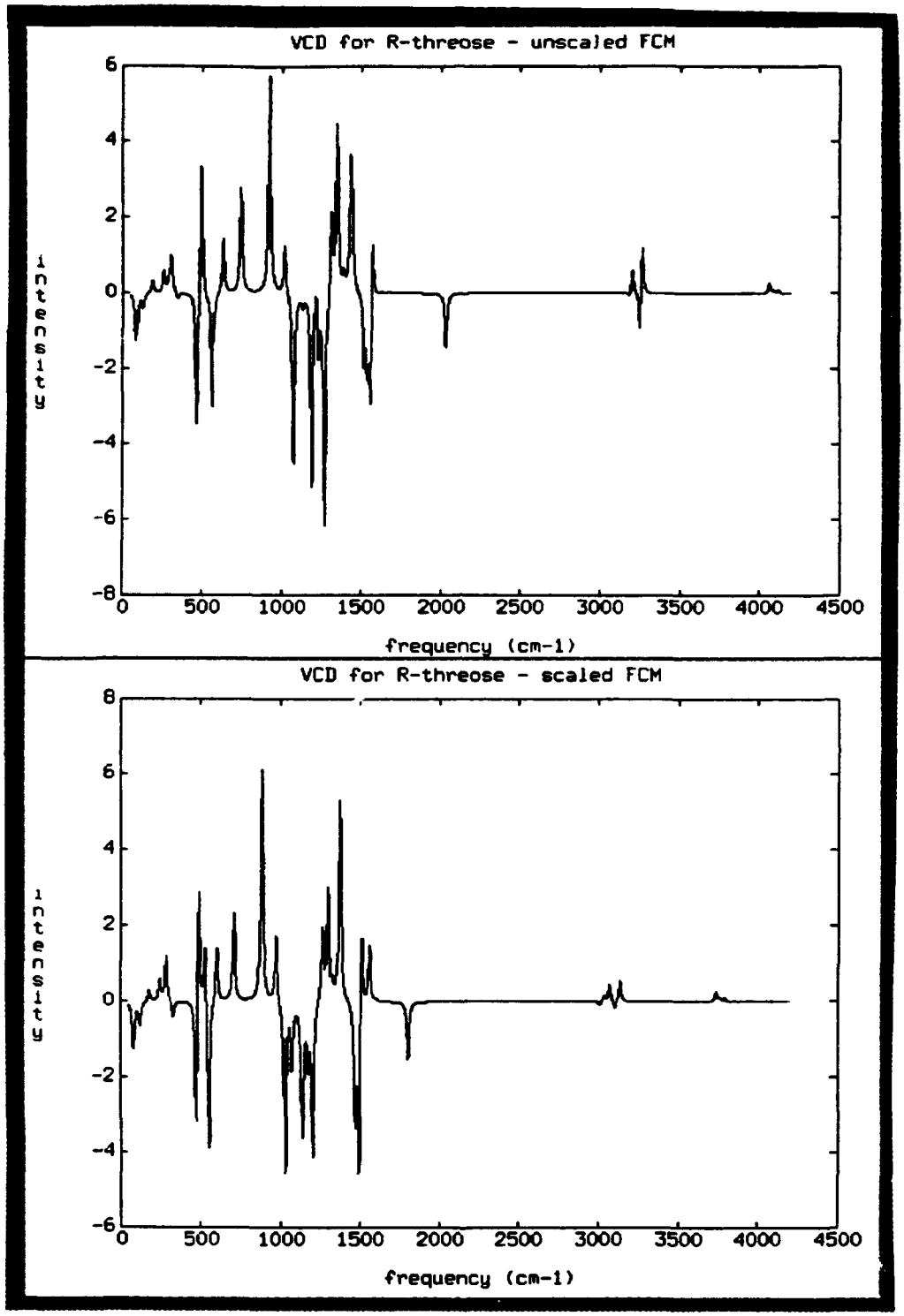
Figure 7. VCD Spectrum of R-Glyceraldehyde [CHO-HCOH-CH_2OH] Based on 6-31G* Level of Calculation: (a) unscaled (b) scaled.



(a)

(b)

Figure 8. VCD Spectrum of R-Erythrose [CHO-HCOH-HCOH-CH_2OH] Based on 6-31G* Level of Calculation: (a) unscaled (b) scaled.



(a)

(b)

Figure 9. VCD Spectrum of R-Threose [CHO-HOCH-HCOH-CH_2OH] Based on 6-31G* Level of Calculation: (a) unscaled (b) scaled.

Table 1a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Formaldehyde [CH_2O] Based on Several Levels of Calculation.

O1

C2

H3 H4

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
geometry					
$r(O_1\text{-}C_2)$/A	1.2069	1.2500	1.1843	1.2200	1.208
$r(C_2\text{-}H_3)$/A	1.0832	1.0994	1.0916	1.1039	1.116
$r(C_2\text{-}C_4)$/A	1.0832	1.0994	1.0916	1.1039	1.116
$\phi(H_3\text{-}C_2\text{-}O_1)$/°	122.5293	122.8893	122.1583	122.1881	121.75
$\phi(H_4\text{-}C_2\text{-}O_1)$/°	122.5293	122.8893	122.1583	122.1881	121.75
$\tau(H_4\text{-}C_2\text{-}O_1\text{-}H_3)$/°	179.9974	179.9999	179.9988	179.9999	180
E/a.u.	-113.221820	-113.443254	-113.866331	-114.174958	-
frequencies (cm^{-1})					
$\tilde{\nu}_1$(CH2 wag)	1337.	1225.	1335.	1213.	1191.
$\tilde{\nu}_2$(CH2 rock)	1378.	1307.	1383.	1297.	1287.
$\tilde{\nu}_3$(CH2 scissors)	1693.	1524.	1680.	1585.	1563.
$\tilde{\nu}_4$(CO str)	1916.	1715.	2028.	1792.	1764.
$\tilde{\nu}_5$(CH2 sym str)	3162.	2986.	3160.	3013.	2944.
$\tilde{\nu}_6$(CH2 asym str)	3233.	3047.	3232.	3085.	3009.

Table 1b. Force Constant Matrix for Formaldehyde [CH_2O] at the 6-31G* HF Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.870968D-01				
2	-0.653834D-06	0.233418D-01			
3	0.122270D-09	0.176079D-05	0.108991D+01		
4	-0.125896D+00	0.563693D-06	-0.165195D-10	0.691419D+00	
5	0.563693D-06	-0.709305D-01	-0.218754D-05	-0.488051D-05	0.215524D+00
6	-0.132665D-10	-0.102660D-05	-0.995841D+00	0.766572D-10	0.436854D-05
7	0.193995D-01	0.501815D-08	-0.172276D-01	-0.282762D+00	0.101694D-05
8	-0.401887D-07	0.237943D-01	0.390051D-06	0.641254D-06	-0.722966D-01
9	-0.436152D-01	0.801975D-07	-0.470322D-01	-0.971029D-01	-0.946715D-07
10	0.193995D-01	0.851225D-07	0.172276D-01	-0.282762D+00	0.329988D-05
11	0.130329D-06	0.237943D-01	0.366984D-07	0.367556D-05	-0.722966D-01
12	0.436152D-01	-0.814386D-06	-0.470322D-01	0.971029D-01	-0.208633D-05

	6	7	8	9	10
6	0.123499D+01				
7	-0.950462D-01	0.284818D+00			
8	-0.696233D-06	-0.128023D-05	0.242539D-01		
9	-0.119573D+00	0.126496D+00	0.162783D-07	0.155489D+00	
10	0.950462D-01	-0.214558D-01	0.679161D-06	0.142221D-01	0.284818D+00
11	-0.264571D-05	0.258271D-06	0.242484D-01	-0.180427D-08	-0.406416D-05
12	-0.119573D+00	-0.142221D-01	0.289903D-06	0.111169D-01	-0.126496D+00

	11	12
11	0.242539D-01	
12	0.261082D-05	0.155489D+00

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.108991D+01				
2	0.396179D-01	0.362177D+00			
3	0.396179D-01	0.570978D-02	0.362177D+00		
4	0.632215D-01	-0.712629D-02	-0.223258D-01	0.332463D+00	
5	0.632215D-01	-0.223258D-01	-0.712629D-02	0.114316D+00	0.332463D+00
6	0.681188D-06	-0.682431D-09	0.145540D-05	-0.123281D-05	-0.195689D-05

	6
6	0.739562D-01

Table 1c. Force Constant Matrix for Formaldehyde [CH_2O] at the 6-31G* MP2 Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.743821D-01				
2	-0.250776D-07	0.186547D-01			
3	0.639575D-12	0.812202D-07	0.836607D+00		
4	-0.110609D+00	0.239689D-07	-0.601145D-12	0.628296D+00	
5	0.723996D-07	-0.573462D-01	-0.126375D-06	-0.270362D-06	0.176320D+00
6	-0.967040D-11	-0.206684D-07	-0.754894D+00	0.724531D-11	0.214100D-06
7	0.181137D-01	-0.760133D-08	-0.131714D-01	-0.258843D+00	0.472538D-07
8	0.566285D-08	0.193465D-01	0.121280D-07	0.820611D-08	-0.594884D-01
9	-0.371663D-01	-0.153492D-07	-0.408557D-01	-0.907064D-01	-0.237975D-07
10	0.181137D-01	0.871074D-08	0.131714D-01	0.258843D+00	0.150708D-06
11	-0.455335D-08	0.193465D-01	0.273618D-09	0.171216D-06	-0.594882D-01
12	0.371663D-01	-0.487996D-07	-0.408557D-01	0.907064D-01	-0.553585D-07

	6	7	8	9	10
6	0.972685D+00				
7	-0.881382D-01	0.260598D+00			
8	-0.527496D-07	-0.444634D-07	0.200728D-01		
9	-0.108896D+00	0.114591D+00	0.484595D-07	0.139383D+00	
10	0.881382D-01	-0.198682D-01	0.303754D-07	0.132815D-01	0.260598D+00
11	-0.132068D-06	0.556931D-08	0.200698D-01	-0.222802D-07	-0.172013D-06
12	-0.108896D+00	-0.132815D-01	-0.103267D-07	0.103685D-01	-0.114591D+00

	11	12
11	0.200728D-01	
12	0.151593D-06	0.139383D+00

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.836603D+00				
2	0.329103D-01	0.329522D+00			
3	0.329103D-01	0.519723D-02	0.329522D+00		
4	0.574901D-01	-0.106197D-01	-0.209151D-01	0.306597D+00	
5	0.574901D-01	-0.209151D-01	-0.106197D-01	0.108957D+00	0.306597D+00
6	0.257913D-07	0.281068D-07	0.101300D-07	0.803072D-08	-0.224167D-06

	6
6	0.625591D-01

Table 1d. Force Constant Scaling Constants, Q(I), and C matrix for Formaldehyde [CH_2O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation.

Q Values

I	Q(I)
1	0.767592E+00
2	0.909836E+00
3	0.909836E+00
4	0.922199E+00
5	0.922199E+00
6	0.845894E+00

C Matrix (6, 6)

		COLUMN 1	COLUMN 2	COLUMN 3
ROW	1	0.1000000000000D+01		
ROW	2	0.9940161605610D+00	0.1000000000000D+01	
ROW	3	0.9940161660580D+00	0.1000435188270+01	0.1000000000000D+01
ROW	4	0.1080812857870+01	0.1626883442350+01	0.1022723080780+01
ROW	5	0.1080812862510+01	0.1022723081800+01	0.1626883222080+01
ROW	6	0.1000000000000D+01	0.1000000000000D+01	0.1000000000000D+01

		COLUMN 4	COLUMN 5	COLUMN 6
ROW	4	0.1000000000000D+01		
ROW	5	0.1033528367550+01	0.1000000000000D+01	
ROW	6	0.1000000000000D+01	0.1000000000000D+01	0.1000000000000D+01

Table 2a. Optimized Geometries, Total Energies and Calculated Wavenumbers ν for Acetaldehyde [C_2H_4O] Based on Several Levels of Calculation.

O3 H4

C7 C2 C1 H5

H6

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
geometry					
$r(C_1\text{-}C_2)$/A	1.5069	1.5232	1.5042	1.5016	-
$r(C_2\text{-}O_3)$/A	1.2085	1.2498	1.1877	1.2225	-
$r(C_1\text{-}H_4)$/A	1.0856	1.0962	1.0866	1.0948	-
$r(C_1\text{-}H_5)$/A	1.0856	1.0962	1.0866	1.0948	-
$r(C_1\text{-}H_6)$/A	1.0856	1.0920	1.0815	1.0901	-
$r(C_2\text{-}C_7)$/A	1.0866	1.1040	1.0952	1.1089	-
$\phi(O_3\text{-}C_2\text{-}C_1)$/°	124.7907	124.8697	124.3941	124.3291	-
$\phi(H_4\text{-}C_1\text{-}C_2)$/°	109.8823	109.8638	109.8144	109.8692	-
$\phi(H_5\text{-}C_1\text{-}C_2)$/°	109.8786	109.8632	109.8130	109.8712	-
$\phi(H_6\text{-}C_1\text{-}C_2)$/°	109.9623	109.1962	110.2725	109.8298	-
$\phi(C_7\text{-}C_2\text{-}C_1)$/°	114.2974	113.7812	115.3303	115.3483	-
$\tau(H_4\text{-}C_1\text{-}C_2\text{-}O_3)$/°	239.1127	239.3247	238.8031	238.8477	-
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}O_3)$/°	120.8851	120.6651	121.1651	121.1716	-
$\tau(H_6\text{-}C_1\text{-}C_2\text{-}O_3)$/°	0.0021	-0.0047	-0.01414	0.0085	-
$\tau(C_7\text{-}C_2\text{-}C_1\text{-}H_4)$/°	59.1128	59.3262	58.8030	58.8444	-
E/a.u.	-152.055249	-152.367295	-152.915966	-153.358969	-

Table 2a. Optimized Geometries, Total Energies and Calculated Wavenumbers ν for Acetaldehyde [C_2H_4O] Based on Several Levels of Calculation. (CONTINUED)

O3 H4

C7 C2 C1 H5

H6

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
frequencies (cm^{-1})					
ν_1	162	171	152	147	
ν_2	531	494	547	52	
ν_3	889	831	856	799	
ν_4	939	883	965	926	
ν_5	1222	1147	1231	1168	
ν_6	1271	1185	1264	1170	
ν_7	1555	1463	1535	1439	
ν_8	1565	1474	1566	1467	
ν_9	1628	1560	1606	1527	
ν_{10}	1645	1579	1616	1535	
ν_{11}	1926	1658	2032	1801	
ν_{12}	3158	2967	3151	2993	
ν_{13}	3200	3087	3206	3107	
ν_{14}	3248	3152	3260	3187	
ν_{15}	3306	3195	3321	3237	

Table 2b. Force Constant Matrix for Acetaldehyde [C_2H_4O] at the 6-31G* HF Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.684061D+00				
2	0.128173D-05	0.593585D+00			
3	-0.146489D-01	-0.140687D-04	0.560879D+00		
4	-0.113158D+00	-0.113777D-06	0.271099D-01	0.107152D+01	
5	0.213922D-05	-0.106715D+00	0.193645D-05	0.101623D-05	0.254940D+00
6	0.321661D-01	0.762112D-05	-0.242137D+00	0.252507D+00	-0.113282D-05
7	0.130304D-02	-0.208682D-05	-0.225147D-01	-0.709047D+00	-0.118767D-06
8	-0.285497D-05	0.298970D-01	-0.312445D-06	-0.370556D-06	-0.768531D-01
9	-0.568162D-01	-0.338779D-06	-0.312980D-01	-0.385271D+00	0.132019D-05
10	-0.124805D+00	0.114489D+00	-0.430063D-01	-0.162294D-02	-0.212717D-02
11	0.113726D+00	-0.239512D+00	0.797452D-01	-0.169873D-02	0.298407D-02
12	-0.430837D-01	0.841654D-01	-0.918934D-01	-0.238752D-01	0.363808D-01
13	-0.124674D+00	-0.114423D+00	-0.429586D-01	-0.162442D-02	0.212352D-02
14	-0.113662D+00	-0.239636D+00	-0.797610D-01	0.169662D-02	0.298563D-02
15	-0.430393D-01	-0.841873D-01	-0.918869D-01	-0.238555D-01	-0.363932D-01
16	-0.325197D+00	-0.664781D-04	0.988285D-01	-0.377124D-03	0.117734D-05
17	-0.663211D-04	-0.598349D-01	0.273003D-04	0.131712D-05	-0.899281D-03
18	0.925477D-01	0.264352D-04	-0.939534D-01	0.450649D-01	0.104439D-04
19	0.247008D-02	0.128105D-05	-0.280988D-02	-0.245691D+00	-0.556418D-06
20	0.132691D-05	0.222167D-01	0.951235D-06	0.266974D-06	-0.764423D-01
21	0.328745D-01	0.219869D-05	-0.971003D-02	0.108320D+00	-0.115167D-06

	6	7	8	9	10
6	0.799925D+00				
7	-0.392920D+00	0.759672D+00			
8	0.132565D-05	0.254960D-06	0.255604D-01		
9	-0.391683D+00	0.451649D+00	-0.111616D-05	0.407673D+00	
10	-0.137515D-02	0.130906D-02	0.124861D-03	-0.145694D-02	0.128097D+00
11	-0.286387D-02	-0.463144D-03	-0.121788D-02	-0.251989D-03	-0.125475D+00
12	-0.548944D-02	0.150130D-03	-0.521762D-02	-0.796009D-02	0.519039D-01
13	-0.137838D-02	0.130836D-02	-0.122181D-03	-0.145637D-02	0.999594D-02
14	0.286035D-02	0.464146D-03	-0.121827D-02	0.251418D-03	-0.152883D-01
15	-0.549135D-02	0.149093D-03	0.521949D-02	-0.795503D-02	0.797526D-02
16	-0.220585D-02	0.309516D-02	0.363011D-06	0.650240D-04	-0.128767D-01
17	-0.301504D-05	0.913752D-06	-0.126280D-02	0.664873D-06	0.282404D-01
18	-0.125502D-01	-0.431321D-02	-0.171686D-05	0.678878D-02	-0.132668D-01
19	0.113206D+00	-0.576412D-01	-0.726729D-07	-0.671366D-02	-0.973231D-04
20	-0.128152D-05	0.358404D-07	0.250947D-01	0.409363D-07	0.358556D-04
21	-0.142574D+00	-0.322009D-01	-0.480546D-07	0.244337D-01	-0.773939D-03

	11	12	13	14	15
11	0.259778D+00				
12	-0.869825D-01	0.929527D-01			
13	0.153074D-01	0.798099D-02	0.127956D+00		
14	-0.244840D-01	-0.113336D-01	0.125401D+00	0.259917D+00	
15	0.113390D-01	0.633414D-02	0.518528D-01	0.870048D-01	0.929443D-01
16	-0.101978D-02	0.505395D-02	-0.128634D-01	0.101138D-02	0.504770D-02
17	0.255094D-02	-0.126595D-01	-0.282501D-01	0.253631D-02	0.126621D-01
18	-0.206297D-02	0.524817D-02	-0.132669D-01	0.205541D-02	0.524818D-02
19	-0.377285D-03	0.186996D-02	-0.980204D-04	0.376704D-03	0.186994D-02
20	-0.998904D-04	-0.435293D-02	-0.369188D-04	-0.100074D-03	0.435503D-02
21	0.107711D-02	0.807890D-03	-0.773591D-03	-0.107742D-02	0.806677D-03

	16	17	18	19	20
16	0.347281D+00				
17	0.739110D-04	0.547147D-01			
18	-0.106299D+00	-0.267514D-04	0.969396D-01		
19	0.938191D-03	-0.776537D-07	-0.466479D-03	0.300119D+00	
20	-0.574033D-06	0.219502D-02	-0.852474D-06	0.742065D-08	0.271358D-01
21	-0.490207D-03	-0.776534D-06	-0.772109D-02	-0.106955D+00	-0.953009D-06

	21
21	0.133957D+00

Table 2b. Force Constant Matrix for Acetaldehyde [C_2H_4O] at the 6-31G* HF Level of Calculation. (CONTINUED)

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.3219090+00				
2	0.447257D-01	0.1068400+01			
3	0.4401790-02	0.934771D-03	0.3723560+00		
4	0.4403330-02	0.9336720-03	0.3414750-02	0.3723490+00	
5	0.2203430-02	0.2334750-02	0.2459220-02	0.2459550-02	0.3863260+00
6	0.7185880-02	0.4095570-01	0.1219540-02	0.1219090-02	0.6278330-05
7	0.4123300-01	-0.1483760-02	0.7282450-02	0.7277500-02	-0.9819160-02
8	0.2433580-01	0.8852390-02	0.1270070-02	-0.9273530-02	-0.8191800-02
9	0.2433050-01	0.8848820-02	-0.9273950-02	0.1271650-02	-0.8192060-02
10	0.2771220-01	-0.2363280-02	-0.8449450-02	-0.8449230-02	-0.1206580-02
11	0.2917800-01	-0.6936370-01	0.1026650-02	0.1028150-02	0.5066840-02
12	-0.8003200-02	-0.9979980-04	0.3372780-02	0.1367160-01	-0.1259440-01
13	0.7998770-02	0.1001500-03	-0.1624850-01	-0.7964570-03	0.1259630-01
14	0.4727840-05	-0.9182820-06	0.1422340-01	-0.1422510-01	-0.7068560-06
15	0.4104060-05	-0.5063060-07	-0.2577260-02	0.2577120-02	-0.5135150-06

	6	7	8	9	10
6	0.3524240+00				
7	-0.179877D-01	0.4984160+00			
8	0.2032370-02	0.2720490-01	0.2371210+00		
9	0.2033840-02	0.2718550-01	0.4202900-01	0.2371090+00	
10	0.6273970-02	-0.3189590-01	0.3602020-01	0.3601950-01	0.2418400+00
11	0.7337060-02	0.2147290+00	-0.7672540-02	-0.7668550-02	0.2854560-01
12	0.4007070-03	-0.7080840-02	0.1804920-01	-0.8142800-01	0.6177600-01
13	-0.4005940-03	0.7078060-02	0.6555000-01	-0.2177160-02	-0.6177020-01
14	-0.8763130-08	-0.1971090-05	-0.6350480-01	0.6350500-01	0.2964750-06
15	-0.1395910-06	-0.1134530-06	-0.1586700-01	0.1587570-01	-0.3087920-05

	11	12	13	14	15
11	0.3497770+00				
12	-0.8573790-03	0.2897720+00			
13	0.8541950-03	-0.1024530+00	0.1949570+00		
14	0.2877280-05	-0.1022500+00	-0.9438500-01	0.2011180+00	
15	0.4447900-05	-0.9488980-01	0.7299720-04	0.7872700-02	0.9496590-01

Table 2c. Force Constant Matrix for Acetaldehyde [C_2H_4O] at the 6-31G* MP2 Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.6392170+00				
2	-0.1322520-05	0.5591830+00			
3	-0.1244260-01	0.1164900-04	0.5106920+00		
4	-0.1031490+00	0.1221150-05	0.2705770-01	0.8775190+00	
5	-0.1863620-06	-0.9148430-01	-0.2512280-05	-0.1516120-04	0.2134860+00
6	0.2829750-01	-0.2317950-05	-0.2240420+00	0.1663070+00	0.6221920-05
7	0.1760910-02	0.1305060-07	-0.2345740-01	-0.5492450+00	0.3709500-05
8	0.8943160-06	0.2501180-01	0.3541070-06	0.2333640-05	-0.6238420-01
9	-0.4930810-01	-0.8166640-06	-0.3028800-01	-0.2877310+00	-0.2839850-06
10	-0.1158390+00	0.1107470+00	-0.4091200-01	-0.1158450-02	-0.1614910-02
11	0.1101320+00	-0.2286020+00	0.7675350-01	-0.1477070-02	0.2756400-02
12	-0.4228890-01	0.8153200-01	-0.8116050-01	-0.2224510-01	0.3159950-01
13	-0.1159140+00	-0.1107850+00	-0.4094180-01	-0.1157820-02	0.1617120-02
14	-0.1101690+00	-0.2285270+00	-0.7674810-01	0.1478730-02	0.2756040-02
15	-0.4231790-01	-0.8152330-01	-0.8116850-01	-0.2225500-01	-0.3159240-01
16	-0.3091340+00	0.3788070-04	0.9248600-01	-0.3015370-03	-0.4488750-06
17	0.3778480-04	-0.5389560-01	-0.1488090-04	-0.1201280-05	-0.1089260-02
18	0.8807050-01	-0.1424540-04	-0.8294980-01	0.4015140-01	-0.5794720-05
19	0.3056930-02	0.2205710-06	-0.1790810-02	-0.2225090+00	0.9823960-05
20	0.1706820-06	0.1831430-01	0.1073670-08	0.1088060-04	-0.6404380-01
21	0.2998870-01	-0.2831810-05	-0.1108470-01	0.9871520-01	-0.4896350-05

	6	7	8	9	10
6	0.6842840+00				
7	-0.2940650+00	0.5931030+00			
8	-0.1502660-05	-0.3431010-05	0.2035300-01		
9	-0.3060080+00	0.3472270+00	0.6063680-06	0.3214270+00	
10	-0.1601750-02	0.9634690-03	-0.7878350-04	-0.1449290-02	0.1194880+00
11	-0.2615390-02	-0.8506660-03	-0.1083730-02	-0.7061780-03	-0.1200290+00
12	-0.7909880-02	0.1249090-02	-0.4171890-02	-0.5850720-02	0.4993990-01
13	-0.1600300-02	0.9639860-03	0.7740530-04	-0.1449570-02	0.8140320-02
14	0.2617270-02	0.8502400-03	-0.1083320-02	0.7068580-03	-0.1479060-01
15	-0.7907210-02	0.1249010-02	0.4170970-02	-0.5853830-02	0.6730040-02
16	-0.1250860-02	0.1699220-02	-0.1847310-06	-0.8390680-03	-0.1117810-01
17	0.1688900-05	-0.2858520-06	-0.1282770-02	-0.3072960-06	0.2574890-01
18	-0.1270370-01	-0.2651240-02	0.1024070-05	0.6534630-02	-0.1227640-01
19	0.1039110+00	-0.4924350-01	0.1851090-05	-0.6449480-02	-0.4162020-03
20	-0.5946100-05	0.5611650-06	0.2047150-01	0.1255280-06	0.1771800-04
21	-0.1257150+00	-0.2955240-01	0.6551040-06	0.2004010-01	-0.4306610-03

	11	12	13	14	15
11	0.2464830+00				
12	-0.8326620-01	0.8453350-01			
13	0.1478060-01	0.6727140-02	0.1195690+00		
14	-0.2155260-01	-0.1064200-01	0.1200700+00	0.2464010+00	
15	0.1063880-01	0.5208100-02	0.4997220-01	0.8325730-01	0.8454130-01
16	-0.2444500-02	0.4985810-02	-0.1118490-01	0.2448640-02	0.4989270-02
17	0.2029440-02	-0.1125070-01	-0.2574370-01	0.2036600-02	0.1124910-01
18	-0.1484630-02	0.4206900-02	-0.1227690-01	0.1488710-02	0.4207270-02
19	-0.1116890-03	0.1632350-02	-0.4160360-03	0.1120080-03	0.1632740-02
20	-0.2986500-04	-0.3800200-02	-0.1730070-04	-0.3018850-04	0.3799100-02
21	0.6802630-03	0.9735500-03	-0.4307940-03	-0.6801540-03	0.9738330-03

	16	17	18	19	20
16	0.3292820+00				
17	-0.4154310-04	0.4988290-01			
18	-0.1001110+00	0.1476460-04	0.8759800-01		
19	0.8161990-03	0.9465560-07	-0.9057660-03	0.2687110+00	
20	0.1618520-06	0.2318940-02	0.1194900-06	-0.1225560-04	0.2299930-01
21	-0.2597600-03	0.2968460-06	-0.6892890-02	-0.9803020-01	0.6651360-05

	21
21	0.1217060+00

Table 2c. Force Constant Matrix for Acetaldehyde [C_2H_4O] at the 6-31G* MP2 Level of Calculation. (CONTINUED)

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.304051D+00				
2	0.394947D-01	0.830117D+00			
3	0.391406D-02	-0.104552D-03	0.353787D+00		
4	0.391325D-02	-0.103821D-03	0.131165D-02	0.353792D+00	
5	0.222062D-02	0.367501D-03	0.536268D-03	0.536148D-03	0.365363D+00
6	0.737696D-02	0.344278D-01	0.582132D-03	0.582290D-03	-0.751155D-04
7	0.368870D-01	-0.361651D-03	0.611013D-02	0.611273D-02	-0.898886D-02
8	0.252019D-01	0.506713D-02	-0.437458D-03	-0.872032D-02	-0.758231D-02
9	0.252028D-01	0.507064D-02	-0.871999D-02	-0.438082D-03	-0.758233D-02
10	0.269544D-01	-0.354849D-02	-0.773000D-02	-0.773038D-02	-0.111160D-03
11	0.298492D-01	-0.645617D-01	0.410264D-03	0.409747D-03	0.492996D-02
12	-0.845426D-02	-0.114775D-02	0.340626D-02	0.136007D-01	-0.123886D-01
13	0.845692D-02	0.114417D-02	-0.159843D-01	-0.102182D-02	0.123874D-01
14	-0.257878D-05	0.526571D-06	0.137004D-01	-0.136996D-01	0.387813D-06
15	-0.151220D-05	0.375466D-05	-0.238414D-02	0.238365D-02	0.284114D-06

	6	7	8	9	10
6	0.317623D+00				
7	-0.140075D-01	0.450485D+00			
8	0.189341D-02	0.235641D-01	0.211947D+00		
9	0.189290D-02	0.235748D-01	0.375080D-01	0.211951D+00	
10	0.472553D-02	-0.281858D-01	0.313792D-01	0.313821D-01	0.218617D+00
11	0.109359D-01	0.191833D+00	-0.758433D-02	-0.758514D-02	0.267034D-01
12	0.713358D-03	-0.692953D-02	0.147247D-01	-0.742022D-01	0.572380D-01
13	-0.714053D-03	0.693673D-02	0.601595D-01	-0.678181D-03	-0.572404D-01
14	-0.677948D-07	0.150825D-05	-0.581993D-01	0.581999D-01	-0.500999D-06
15	0.651123D-06	-0.464727D-05	-0.140484D-01	0.140449D-01	0.710957D-07

	11	12	13	14	15
11	0.319669D+00				
12	-0.778527D-03	0.261148D+00			
13	0.783518D-03	-0.939791D-01	0.178662D+00		
14	-0.109386D-05	-0.955460D-01	-0.870292D-01	0.187326D+00	
15	-0.539959D-05	-0.824865D-01	0.294517D-05	0.851039D-02	0.824877D-01

Table 2d. Force Constant Scaling Constants, Q(I), and C matrix for Acetaldehyde [C_2H_4O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation.

Q Values

I	Q(I)
1	0.944523E+00
2	0.776971E+00
3	0.950131E+00
4	0.950162E+00
5	0.945737E+00
6	0.901252E+00
7	0.903834E+00
8	0.893833E+00
9	0.893899E+00
10	0.903976E+00
11	0.913922E+00
12	0.901219E+00
13	0.916417E+00
14	0.931421E+00
15	0.868603E+00

C Matrix (15,15)

		COLUMN 1	COLUMN 2	COLUMN 3
ROW	1	0.1000000000000+01		
ROW	2	0.1030795274650+01	0.1000000000000D+01	
ROW	3	0.9386423687850+00	0.1000000000000+01	0.1000000000000+01
ROW	4	0.9381055447140+00	0.1000000000000+01	0.4042664868270+00
ROW	5	0.1066310486630+01	0.1836241662920+00	0.2300420547520+00
ROW	6	0.1112673929090+01	0.1004546842280+01	0.5158366943330+00
ROW	7	0.9682286236270+00	0.2908574633440+00	0.9053925154850+00
ROW	8	0.1127078279320+01	0.6868649952400+00	-0.3737575152250+00
ROW	9	0.1127323764210+01	0.6875918885100+00	0.1020269979350+01
ROW	10	0.1052623080060+01	0.1791625637950+01	0.9871450514730+00
ROW	11	0.1101071248530+01	0.1104550754340+01	0.4288392288270+00
ROW	12	0.1144959691830+01	0.1000000000000+01	0.1091397384960+01
ROW	13	0.1136412414050+01	0.1000000000000+01	0.1054248123880+01
ROW	14	0.1000000000000+01	0.1000000000000+01	0.1023917866650+01
ROW	15	0.1000000000000+01	0.1000000000000+01	0.1018290125840+01

		COLUMN 4	COLUMN 5	COLUMN 6
ROW	4	0.1000000000000+01		
ROW	5	0.2299562794560+00	0.1000000000000+01	
ROW	6	0.5161567817750+00	0.1000000000000+01	0.1000000000000+01
ROW	7	0.9063787530310+00	0.9901498413170+00	0.8628135148260+00
ROW	8	0.1020376508100+01	0.1006720284690+01	0.1037982750220+01
ROW	9	-0.3738041726360+00	0.1006653971170+01	0.1036915412540+01
ROW	10	0.9872029159690+00	0.9963952986680-01	0.8344614922890+00
ROW	11	0.4276675023240+00	0.1046563215250+01	0.1642306167460+01
ROW	12	0.1075047943660+01	0.1065478478970+01	0.1000000000000+01
ROW	13	0.1000000000000+01	0.1056348811460+01	0.1000000000000+01
ROW	14	0.1023720717970+01	0.1000000000000+01	0.1000000000000+01
ROW	15	0.1018117537850+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 7	COLUMN 8	COLUMN 9
ROW	7	0.1000000000000+01		
ROW	8	0.9636760992090+00	0.1000000000000+01	
ROW	9	0.9647669694670+00	0.9983959193830+00	0.1000000000000+01
ROW	10	0.9776280830850+00	0.9691471249910+00	0.9692193650830+00
ROW	11	0.9829551547200+00	0.1093693831900+01	0.1094337990090+01
ROW	12	0.1084325631700+01	0.9089623647930+00	0.1015275186850+01
ROW	13	0.1076837617090+01	0.1014045077810+01	0.3441635713390+00
ROW	14	0.1000000000000+01	0.1004081679000+01	0.1004377665320+01
ROW	15	0.1000000000000+01	0.1004832907760+01	0.1003995640850+01

Table 2d. Force Constant Scaling Constants, Q(I), and C matrix for Acetaldehyde [C_2H_4O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED)

		COLUMN 10	COLUMN 11	COLUMN 12
ROW	10	0.1000000000000+01		
ROW	11	0.1029185959910+01	0.1000000000000+01	
ROW	12	0.1026530331500+01	0.1000000000000+01	0.1000000000000+01
ROW	13	0.1018119419980+01	0.1000000000000+01	0.1009352622820+01
ROW	14	0.1000000000000+01	0.1000000000000+01	0.1019912688580+01
ROW	15	0.1000000000000+01	0.1000000000000+01	0.9825120012670+00

		COLUMN 13	COLUMN 14	COLUMN 15
ROW	13	0.1000000000000+01		
ROW	14	0.9980269837240+00	0.1000000000000+01	
ROW	15	0.1000000000000+01	0.1201826438550+01	0.1000000000000+01

Table 3a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Methanol [CH_3OH] Based on Several Levels of Calculation.

H2

H3 C1 O5 H6

H4

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
geometry					
$r(C_1\text{-}H_2)$/A	1.0851	1.0980	1.0874	1.0968	
$r(C_1\text{-}H_3)$/A	1.0851	1.0980	1.0874	1.0968	
$r(C_1\text{-}H_4)$/A	1.0786	1.0903	1.0811	1.0896	
$r(C_1\text{-}O_5)$/A	1.4409	1.4709	1.3996	1.4229	
$r(O_5\text{-}H_6)$/A	0.9658	0.9915	0.9463	0.9700	
$\phi(H_3\text{-}C_1\text{-}H_2)$/°	108.7459	108.4380	108.6812	108.7703	
$\phi(H_4\text{-}C_1\text{-}H_2)$/°	108.6009	108.4942	108.3925	108.4878	
$\phi(O_5\text{-}C_1\text{-}H_2)$/°	112.2366	112.8587	112.0363	112.3174	
$\phi(H_6\text{-}O_5\text{-}C_1)$/°	110.3343	107.0565	109.4474	107.4264	
$\tau(H_4\text{-}C_1\text{-}H_2\text{-}H_3)$/°	241.9887	242.3481	242.3911	242.176	
$\tau(O_5\text{-}C_1\text{-}H_2\text{-}H_3)$/°	124.7839	125.7980	124.3429	124.9632	
$\tau(H_6\text{-}O_5\text{-}C_1\text{-}H_2)$/°	-61.4165	-61.6912	-61.2228	-61.5056	
E/a.u.	-114.398019	-114.612722	-115.035418	-115.353295	-

Table 3a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Methanol [CH_3OH] Based on Several Levels of Calculation. (CONTINUED)

H2

H3 C1 O5 H6

H4

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
frequencies (cm^{-1})					
$\tilde{\nu}_1$(torsion)	360	380	348	352	295
$\tilde{\nu}_2$(CO str)	1090	990	1164	1085	1033
$\tilde{\nu}_3$(CH3 rock)	1153	1098	1189	1114	1060
$\tilde{\nu}_4$(CH3 rock)	1254	1181	1290	1205	1165
$\tilde{\nu}_5$(OH bend)	1480	1417	1508	1418	1345
$\tilde{\nu}_6$(CH3 s-deform)	1638	1555	1638	1540	1455
$\tilde{\nu}_7$(CH3 d-deform)	1686	1606	1652	1566	1477
$\tilde{\nu}_8$(CH3 d-deform)	1698	1623	1663	1580	1477
$\tilde{\nu}_9$(CH3 s-str)	3179	3050	3185	3077	2844
$\tilde{\nu}_{10}$(CH3-d-str)	3218	3094	3231	3144	2960
$\tilde{\nu}_{11}$(CH3-d-str)	3294	3183	3305	3223	3000
ν_{12}(OH str)	3868	3521	4118	3798	3681

Table 3b. Force Constant Matrix for Methanol [CH_3OH] at the 6-31G* HF Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.6417790+00				
2	-0.4999490-01	0.6420460+00			
3	-0.2528970-02	-0.3587470-01	0.6434920+00		
4	-0.6613600-01	0.1396060-02	0.1208730-01	0.6284870-01	
5	0.3491540-02	-0.6625150-01	0.1706320-01	0.6722390-02	0.6709050-01
6	0.8906390-02	0.1278470-01	-0.3339400+00	-0.2847980-02	-0.3936580-02
7	-0.3000940+00	0.1255940-01	0.8801180-01	0.1645460-02	0.1536140-02
8	0.1728250-01	-0.6625160-01	-0.2157850-02	-0.2013840-02	0.2904600-02
9	0.9119190-01	-0.2772470-02	-0.9998120-01	0.3693010-01	-0.2645450-02
10	-0.1286720+00	0.1214980+00	-0.4572560-01	0.2501970-02	-0.2491730-02
11	0.1085780+00	-0.2542090+00	0.7790380-01	0.7874960-03	0.2085710-02
12	-0.4572520-01	0.8717370-01	-0.9775110-01	-0.1867560-01	0.3172340-01
13	-0.1572490+00	-0.5487150-01	-0.5929500-01	-0.9858180-03	-0.9897640-02
14	-0.9894150-01	-0.2231600+00	-0.7098950-01	-0.8169150-02	-0.8043750-02
15	-0.5929190-01	-0.3936410-01	-0.1171570+00	-0.2841860-01	-0.4113800-01
16	0.1037260-01	-0.3058670-01	0.7450560-02	0.1257610-03	0.6393040-03
17	0.1958440-01	-0.3217340-01	0.1405500-01	0.1277050-02	0.2214400-02
18	0.7447760-02	-0.2194710-01	0.5337770-02	0.9247970-03	-0.1066620-02

	6	7	8	9	10
6	0.3659300+00				
7	0.1875120-02	0.3331060+00			
8	0.2302490-02	-0.1576860-02	0.6709040-01		
9	-0.1147530-01	-0.9422680-01	0.7628900-02	0.9567110-01	
10	0.1171080-02	-0.1445260-01	0.2925380-01	-0.1294290-01	0.1292250+00
11	0.1848350-02	0.2003450-02	0.2085520-02	0.1542250-03	-0.1164070+00
12	-0.1047230-01	0.6903900-02	-0.1252160-01	0.6482380-02	0.5165580-01
13	-0.8865620-02	-0.2055800-01	-0.4214000-01	-0.2179990-01	0.1317270-01
14	-0.1301210-01	-0.1494360-01	-0.8042720-02	-0.3570360-02	-0.2651140-01
15	-0.1018990-01	-0.2247860-02	0.3800830-02	0.9383410-02	0.7483770-02
16	-0.2389940-03	0.3534800-03	-0.8056610-03	0.8476350-03	-0.1774160-02
17	0.1321480-04	0.4215300-03	0.2213850-02	0.1205150-02	-0.5341150-02
18	0.1481710-03	-0.3161000-03	0.9472300-03	-0.8038350-04	-0.1642220-02

	11	12	13	14	15
11	0.2908600+00				
12	-0.8352220-01	0.9429200-01			
13	0.9580870-02	0.7482980-02	0.3055060+00		
14	-0.3759620-01	-0.1902100-01	-0.7656170-01	0.7223480+00	
15	0.6875900-02	0.8112710-02	0.1803010+00	-0.5498280-01	0.1836340+00
16	-0.4542450-02	-0.1641950-02	-0.1398860+00	0.2251270+00	-0.9782620-01
17	-0.3226010-02	-0.3832210-02	0.1738900+00	-0.4455050+00	0.1248080+00
18	-0.3260050-02	-0.6637760-03	-0.9782310-01	0.1615760+00	-0.7378370-01

	16	17	18
16	0.1308080+00		
17	-0.1898320+00	0.4764760+00	
18	0.9140890-01	-0.1362490+00	0.6904190-01

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.3659300+00				
2	0.5451910-02	0.3659290+00			
3	0.4343490-02	0.4343650-02	0.3847760+00		
4	0.1847750-01	0.1847800-01	0.1210660-01	0.4285660+00	
5	-0.6606890-04	-0.6632690-04	-0.2303180-02	-0.2859270-02	0.6087050+00
6	0.2110490-01	0.5853040-02	-0.1120930-01	-0.3296180-01	0.1592450-02
7	0.1959510-01	-0.1256070-01	0.2780730-02	-0.3328700-01	-0.3664830-02
8	0.8809580-02	-0.4139180-02	-0.5666590-02	-0.2025120-02	-0.5675780-02
9	0.1541180-03	0.1544750-03	0.4015280-02	0.4771380-01	0.1629150-01
10	0.3672230-02	-0.1473690-01	-0.4373440-02	0.5235650-01	0.5763910-02
11	0.8100510-03	0.7072640-02	-0.9565260-02	-0.3421360-02	-0.9578580-02
12	0.4379440-03	-0.4372510-03	-0.4976950-06	-0.1296720-05	0.7873210-06

	6	7	8	9	10
6	0.2654040+00				
7	0.4456550-01	0.2557080+00			
8	0.8353960-01	0.7055310-01	0.3547520+00		
9	0.4410220-02	-0.1592300-01	-0.1697340-01	0.2052400+00	
10	0.5816890-01	-0.2652270-01	-0.8162220-01	0.2504510-01	0.2567850+00
11	-0.8505990-01	0.8846970-01	-0.1301840-03	-0.2864850-01	-0.1553110+00
12	0.2350090-02	-0.1516270-02	-0.2487400-02	-0.1074020-05	-0.8703750-03

	11	12
11	0.3080860+00	
12	0.4938830-02	0.9781450-02

Table 3c. Force Constant Matrix for Methanol [CH_3OH] at the 6-31G* MP2 Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.5879090+00				
2	-0.5868590-01	0.5790280+00			
3	-0.9716470-02	-0.4203120-01	0.5945050+00		
4	-0.5864470-01	0.1548710-02	0.1114900-01	0.5659700-01	
5	0.3217960-02	-0.5792390-01	0.1518260-01	0.5518350-02	0.5908280-01
6	0.9157310-02	0.1322270-01	-0.3171350+00	-0.3366880-02	-0.4865280-02
7	-0.2841880+00	0.1301570-01	0.8580680-01	0.1090300-02	0.1767550-02
8	0.1541020-01	-0.5792420-01	-0.1839400-02	-0.1705560-02	0.2608390-02
9	0.8779960-01	-0.2789540-02	-0.9159510-01	0.3343410-01	-0.2402120-02
10	-0.1191100+00	0.1173010+00	-0.4403970-01	0.2009250-02	-0.2147300-02
11	0.1069300+00	-0.2404450+00	0.7659770-01	0.9194630-03	0.1810360-02
12	-0.4404030-01	0.8402700-01	-0.8917610-01	-0.1691150-01	0.2873240-01
13	-0.1314890+00	-0.4325200-01	-0.4758770-01	-0.7957980-03	-0.8465240-02
14	-0.8516240-01	-0.1914210+00	-0.6100350-01	-0.7859230-02	-0.7787250-02
15	-0.4759420-01	-0.3099500-01	-0.9913150-01	-0.2499100-01	-0.3526810-01
16	0.5520560-02	-0.2992790-01	0.4388070-02	-0.2551490-03	0.1083590-03
17	0.1828930-01	-0.3131650-01	0.1309350-01	0.1578040-02	0.2210240-02
18	0.4394200-02	-0.2143390-01	0.2531500-02	0.6859010-03	-0.1379560-02

	6	7	8	9	10
6	0.3442510+00				
7	0.2847780-04	0.3124190+00			
8	0.2446500-02	-0.2830620-02	0.5908230-01		
9	-0.1028160-01	-0.9030790-01	0.6790690-02	0.8843190-01	
10	0.2093980-02	-0.1244790-01	0.2651340-01	-0.1199830-01	0.1206000+00
11	0.1843440-03	0.4698780-03	0.1810710-02	0.8108800-03	-0.1123500+00
12	-0.9082350-02	0.7007000-02	-0.1127860-01	0.5374940-02	0.4939170-01
13	-0.7284800-02	-0.1711250-01	-0.3611620-01	-0.1944590-01	0.1021900-01
14	-0.1153140-01	-0.1344470-01	-0.7788040-02	-0.3730220-02	-0.2397060-01
15	-0.8027690-02	-0.1738320-02	0.3333830-02	0.8287820-02	0.5915570-02
16	-0.6277010-03	0.2391770-03	-0.1271370-02	0.5181490-03	-0.1270920-02
17	0.5431440-03	0.1022110-02	0.2211480-02	0.1320140-02	-0.5346690-02
18	0.2753670-03	-0.7954580-03	0.5466280-03	-0.2171170-03	-0.1363500-02

	11	12	13	14	15
11	0.2728970+00				
12	-0.8047880-01	0.8703080-01			
13	0.7654610-02	0.5917200-02	0.2617400+00		
14	-0.3247350-01	-0.1717200-01	-0.6828410-01	0.6073930+00	
15	0.5479850-02	0.6196740-02	0.1535410+00	-0.4881230-01	0.1572620+00
16	-0.3623490-02	-0.1364170-02	-0.1225620+00	0.1987200+00	-0.8513350-01
17	-0.3599890-02	-0.3830040-02	0.1484640+00	-0.3679240+00	0.1062630+00
18	-0.2593430-02	-0.3437580-03	-0.8514030-01	0.1422490+00	-0.6458640-01

	16	17	18
16	0.1183290+00		
17	-0.1640060+00	0.3984190+00	
18	0.8221940-01	-0.1173890+00	0.6234010-01

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.3442510+00				
2	0.3335330-02	0.3442540+00			
3	0.2107660-02	0.2107190-02	0.3644680+00		
4	0.1546910-01	0.1546690-01	0.9673920-02	0.3722420+00	
5	-0.6461310-03	-0.6454540-03	-0.1804390-02	-0.5867620-02	0.5176170+00
6	0.2015740-01	0.6978200-02	-0.1086860-01	-0.3015030-01	0.2567800-02
7	0.1826760-01	-0.1209950-01	0.3021040-02	-0.3116310-01	-0.4318240-02
8	0.5183940-02	-0.2256750-02	-0.4856370-02	-0.2870460-02	-0.6606970-02
9	0.1906070-04	0.1820260-04	0.3368550-02	0.5428420-01	0.1831170-01
10	0.3784380-02	-0.1351910-01	-0.4769300-02	0.4918860-01	0.6817130-02
11	0.1016300-02	0.3971080-02	-0.8271950-02	-0.4892520-02	-0.1125950-01
12	0.1030570-02	-0.1032490-02	0.1437540-05	0.3700530-05	-0.1757830-05

	6	7	8	9	10
6	0.2431260+00				
7	0.4052820-01	0.2333330+00			
8	0.7550450-01	0.6191470-01	0.3158960+00		
9	0.3788880-02	-0.1479220-01	-0.1490130-01	0.1948440+00	
10	0.5326410-01	-0.2265220-01	-0.7334690-01	0.2334770-01	0.2327140+00
11	-0.7570240-01	0.7968980-01	0.2160120-03	-0.2538910-01	-0.1396310+00
12	0.2558560-02	-0.1957230-02	-0.2289410-02	0.3068480-05	-0.1108950-02

	11	12
11	0.2740490+00	
12	0.5184130-02	0.1064290-01

Table 3d. Force Constant Scaling Constants, Q(I), and C matrix for Methanol [CH_3OH] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation.

Q Values

I	Q(I)
1	0.940758E+00
2	0.940768E+00
3	0.947221E+00
4	0.868576E+00
5	0.850357E+00
6	0.916061E+00
7	0.912498E+00
8	0.890468E+00
9	0.949345E+00
10	0.906260E+00
11	0.889519E+00
12	0.108807E+01

C Matrix (12,12)

		COLUMN 1	COLUMN 2	COLUMN 3
ROW	1	0.1000000000000D+01		
ROW	2	0.6502954116590D+00	0.1000000000000D+01	
ROW	3	0.5140403461000D+00	0.5139045937630D+00	0.1000000000000D+01
ROW	4	0.9261413631490D+00	0.9259810514700D+00	0.8809529547980D+00
ROW	5	0.1000000000000D+01	0.1000000000000D+01	0.8729247701520D+00
ROW	6	0.1028846760920D+01	0.1284276659180D+01	0.1040896206120D+01
ROW	7	0.1006190377090D+01	0.1039670405330D+01	0.1168574427710D+01
ROW	8	0.6429198925480D+00	0.5956862918470D+00	0.9331567929320D+00
ROW	9	0.1000000000000D+01	0.1000000000000D+01	0.8846857686330D+00
ROW	10	0.1116090528640D+01	0.9935180158590D+00	0.1177006874620D+01
ROW	11	0.1000000000000D+01	0.6137725388290D+00	0.9421234022920D+00
ROW	12	0.1000000000000D+01	0.1000000000000D+01	0.1000000000000D+01

		COLUMN 4	COLUMN 5	COLUMN 6
ROW	4	0.1000000000000D+01		
ROW	5	0.2387824585050D+01	0.1000000000000D+01	
ROW	6	0.1025450557200D+01	0.1826977911720D+01	0.1000000000000D+01
ROW	7	0.1051591939140D+01	0.1337633179980D+01	0.9946721727300D+00
ROW	8	0.1611711606830D+01	0.1337724677030D+01	0.1000712571710D+01
ROW	9	0.1252889702710D+01	0.1250995808390D+01	0.9212478106240D+00
ROW	10	0.1058919393620D+01	0.1347279287550D+01	0.1004973683510D+01
ROW	11	0.1626867446280D+01	0.1351579544440D+01	0.9859269339160D+00
ROW	12	0.1000000000000D+01	0.1000000000000D+01	0.1090489911990D+01

		COLUMN 7	COLUMN 8	COLUMN 9
ROW	7	0.1000000000000D+01		
ROW	8	0.9735383332600D+00	0.1000000000000D+01	
ROW	9	0.9981091744100D+00	0.9548449126220D+00	0.1000000000000D+01
ROW	10	0.9391810170590D+00	0.1000317132650D+01	0.1005038582880D+01
ROW	11	0.9998041162340D+00	0.1000000000000D+01	0.9643989838570D+00
ROW	12	0.1295452731180D+01	0.9350635795930D+00	0.1000000000000D+01

		COLUMN 10	COLUMN 11	COLUMN 12
ROW	10	0.1000000000000D+01		
ROW	11	0.1001324380010+01	0.1000000000000D+01	
ROW	12	0.1000000000000D+01	0.1066957376500+01	0.1000000000000D+01

Table 4a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Ethanol [C_2H_6O] Based on Several Levels of Calculation.

H4 H8

H5 C1 C2 O3 H9

H6 H7

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
geometry					
$r(C_1\text{-}C_2)$/A	1.5315	1.5413	1.5214	1.5183	-
$r(C_2\text{-}O_3)$/A	1.4435	1.4737	1.4037	1.4270	-
$r(C_2\text{-}H_4)$/A	1.0837	1.0946	1.0860	1.0940	-
$r(C_1\text{-}H_5)$/A	1.0856	1.0962	1.0874	1.0947	-
$r(C_1\text{-}H_6)$/A	1.0825	1.0930	1.0844	1.0918	-
$r(C_2\text{-}H_7)$/A	1.0852	1.0990	1.0885	1.0991	-
$r(C_2\text{-}H_8)$/A	1.0788	1.0914	1.0821	1.0920	-
$r(O_3\text{-}H_9)$/A	0.9666	0.9930	0.9472	0.9717	-
$\phi(O_3\text{-}C_2\text{-}C_1)$/°	111.6631	111.7738	112.4790	111.2820	-
$\phi(H_4\text{-}C_1\text{-}C_2)$/°	110.7423	110.7753	110.8558	111.0791	-
$\phi(H_5\text{-}C_1\text{-}C_2)$/°	110.8086	110.5287	111.0359	110.7650	-
$\phi(H_6\text{-}C_1\text{-}C_2)$/°	109.5821	109.2399	110.3870	109.9832	-
$\phi(H_7\text{-}C_2\text{-}C_1)$/°	110.2965	110.0987	110.2863	110.4819	-
$\phi(H_8\text{-}C_2\text{-}C_1)$/°	110.2823	110.2315	110.2089	110.5177	-
$\phi(H_9\text{-}O_3\text{-}C_2)$/°	110.1141	106.5869	109.3783	107.0600	-
$\tau(H_4\text{-}C_1\text{-}C_2\text{-}O_3)$/°	184.6308	185.1689	182.4335	183.1188	-
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}O_3)$/°	64.5741	65.1689	62.6959	63.3273	-
$\tau(H_6\text{-}C_1\text{-}C_2\text{-}O_3)$/°	-55.0392	-54.3060	-57.1645	-56.3440	-
$\tau(H_7\text{-}C_2\text{-}C_1\text{-}H_4)$/°	60.5775	60.3535	-58.4414	58.7372	-
$\tau(H_8\text{-}C_2\text{-}C_1\text{-}H_4)$/°	-58.7615	-58.9067	59.8060	-59.9815	-
$\tau(H_9\text{-}O_3\text{-}C_2\text{-}C_1)$/°	-62.6293	-62.0978	-64.0085	-62.7393	-
E/a.u.	-153.222920	-153.530203	-154.075576	-154.529909	-

Table 4a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Ethanol [C_2H_6O] Based on Several Levels of Calculation. (CONTINUED)

H4 H8

H5 C1 C2 O3 H9

H6 H7

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
frequencies (cm^{-1})					
$\tilde{\nu}_1$	270	275	278	285	
ν_2	336	352	328	329	
ν_3	423	393	453	430	
ν_4	891	842	868	829	
ν_5	933	880	966	923	
ν_6	1110	1035	1150	1099	
ν_7	1156	1098	1195	1120	
ν_8	1234	1167	1246	1174	
ν_9	1411	1351	1400	1327	
ν_{10}	1496	1424	1509	1418	
ν_{11}	1537	1454	1546	1450	
ν_{12}	1571	1490	1578	1476	
ν_{13}	1663	1595	1634	1556	
ν_{14}	1671	1602	1640	1561	
ν_{15}	1693	1618	1673	1585	
ν_{16}	3189	3056	3185	3077	
ν_{17}	3198	3087	3198	3105	
ν_{18}	3248	3147	3250	3175	
ν_{19}	3277	3168	3277	3193	
ν_{20}	3290	3182	3287	3214	
ν_{21}	3859	3503	4104	3772	

Table 4b. Force Constant Matrix for Ethanol [C_2H_6O] at the 6-31G* HF Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.658442D+00				
2	0.616476D-02	0.648335D+00			
3	-0.151241D-02	-0.233527D-02	0.559353D+00		
4	-0.954646D-01	-0.185072D-03	0.995322D-02	0.612619D+00	
5	0.208023D-02	-0.104214D+00	0.103725D-02	-0.175013D-01	0.724054D+00
6	0.235464D-01	-0.549377D-03	-0.236385D+00	-0.422683D-01	0.179577D-01
7	-0.173340D-01	0.208389D-02	-0.937067D-02	-0.262170D+00	-0.221623D-01
8	-0.351804D-03	0.505727D-02	-0.110349D-02	0.233039D-01	-0.112815D+00
9	-0.549318D-01	0.534067D-03	-0.156002D-01	-0.582175D-01	-0.257046D-01
10	-0.307778D+00	0.104215D-01	-0.942858D-01	0.137308D-02	-0.281137D-03
11	0.106311D-01	-0.591276D-01	0.456232D-02	0.473076D-04	-0.183621D-02
12	-0.911560D-01	0.448480D-02	-0.967929D-01	-0.382555D-01	0.192933D-02
13	-0.110616D+00	0.987316D-01	0.423215D-01	-0.164099D-02	0.480543D-03
14	0.995078D-01	-0.254058D+00	-0.809410D-01	0.260155D-03	0.144213D-02
15	0.408525D-01	-0.799247D-01	-0.936470D-01	0.199831D-01	-0.373293D-01
16	-0.134561D+00	-0.115974D+00	0.513359D-01	-0.136620D-02	-0.412792D-03
17	-0.116014D+00	-0.241531D+00	0.784559D-01	0.697552D-04	0.153698D-02
18	0.483986D-01	0.761004D-01	-0.919106D-01	0.234414D-01	0.346792D-01
19	0.304146D-02	-0.112803D-02	0.914216D-03	-0.124129D+00	-0.957049D-01
20	0.831837D-03	0.196554D-02	-0.191396D-02	-0.101316D+00	-0.237906D+00
21	0.196666D-01	0.335231D-01	-0.130282D-01	0.498799D-01	0.768949D-01
22	0.206049D-02	0.223255D-03	0.592092D-03	-0.105590D+00	0.884883D-01
23	-0.151563D-02	0.289946D-02	0.142610D-02	0.101448D+00	-0.271573D+00
24	0.163587D-01	-0.346010D-01	-0.131627D-01	0.471976D-01	-0.876444D-01
25	0.220886D-02	-0.338039D-03	0.519513D-04	-0.236312D-01	0.450133D-01
26	-0.133435D-02	0.673763D-03	0.812172D-03	-0.612689D-02	0.131211D-02
27	-0.122264D-02	0.276795D-02	0.117399D-02	-0.117140D-01	0.181799D-01

	6	7	8	9	10
6	0.575244D+00				
7	-0.872272D-01	0.498540D+00			
8	-0.679865D-02	-0.216396D+00	0.533682D+00		
9	-0.113697D+00	0.677667D-01	0.160071D+00	0.175183D+00	
10	0.306553D-02	0.151902D-02	0.225559D-03	-0.104471D-02	0.333276D+00
11	0.718985D-04	-0.176532D-03	0.185170D-02	-0.122633D-03	-0.120554D-01
12	-0.316605D-02	-0.352161D-02	-0.121794D-03	-0.116199D-01	0.103956D+00
13	-0.145548D-02	0.181954D-02	-0.135433D-02	0.668470D-03	-0.137762D-01
14	0.209009D-02	-0.243555D-02	0.107263D-02	-0.224307D-03	0.566741D-03
15	-0.126089D-01	0.197165D-03	0.189708D-02	0.413230D-02	-0.475012D-02
16	-0.126794D-02	0.181942D-02	0.941600D-03	0.471246D-03	-0.158118D-01
17	-0.147746D-02	0.185294D-02	0.431876D-03	-0.151027D-03	0.151241D-02
18	-0.131936D-01	-0.813464D-03	-0.207234D-02	0.476380D-02	-0.591972D-02
19	0.502153D-01	-0.404370D-01	-0.305980D-01	0.150940D-02	0.503264D-03
20	0.758299D-01	-0.252441D-02	0.964035D-02	-0.375505D-02	0.258846D-03
21	-0.100927D+00	-0.158617D-01	-0.150310D-01	0.820141D-02	-0.944969D-03
22	0.413950D-01	-0.304029D-01	0.390953D-01	0.849002D-02	0.430258D-03
23	-0.846893D-01	0.329221D-02	0.394375D-02	0.225368D-02	-0.312452D-03
24	-0.997866D-01	-0.123259D-01	0.162414D-01	0.711644D-02	-0.807769D-03
25	0.139967D-01	-0.153354D+00	0.185134D+00	0.352882D-01	0.263670D-03
26	-0.243480D-02	0.236466D+00	-0.442864D+00	-0.132901D+00	-0.336096D-03
27	0.452083D-02	0.611567D-01	-0.153082D+00	-0.584798D-01	0.731702D-03

	11	12	13	14	15
11	0.555004D-01				
12	-0.424579D-02	0.982874D-01			
13	0.302853D-01	0.134404D-01	0.112860D+00		
14	0.100210D-04	0.888864D-03	-0.111756D+00	0.272419D+00	
15	0.128614D-01	0.541967D-02	-0.469496D-01	0.900347D-01	0.989423D-01
16	-0.281376D-01	0.129622D-01	0.103138D-01	0.139418D-01	-0.731186D-02
17	0.354438D-02	-0.252096D-02	-0.161955D-01	-0.236615D-01	0.105690D-01
18	-0.125885D-01	0.526798D-02	-0.826135D-02	-0.102802D-01	0.491462D-02
19	0.441257D-05	0.119304D-02	-0.328523D-03	-0.183620D-03	-0.284157D-03
20	-0.895191D-04	0.934127D-03	-0.344319D-04	0.116022D-02	0.852502D-03
21	-0.155209D-03	0.128273D-02	0.332551D-03	-0.969785D-03	0.206282D-02

Table 4b. Force Constant Matrix for Ethanol [C_2H_6O] at the 6-31G* HF Level of Calculation. (CONTINUED 1)

22	-0.1486800-03	0.6353850-03	0.1095820-02	0.2614410-03	-0.4199190-03
23	0.1491010-04	-0.9480780-03	-0.5204080-03	0.1842390-02	0.7547170-03
24	0.2399800-03	0.1457790-02	-0.4678950-04	0.5444780-03	-0.8394920-02
25	-0.4499980-03	0.7461970-03	0.2721420-03	-0.1630390-03	-0.1317160-02
26	0.1320010-03	-0.4004980-03	0.3629190-03	-0.2264330-03	0.2846740-03
27	-0.6234770-03	-0.1367200-03	-0.4972990-04	-0.1142860-02	-0.8208290-03

	16	17	18	19	20
16	0.1387850+00				
17	0.1289640+00	0.2572140+00			
18	-0.5642160-01	-0.8507990-01	0.9705520-01		
19	0.1119950-02	-0.1719670-03	-0.4053630-03	0.1475280+00	
20	0.4480290-03	0.1789260-02	-0.3580490-03	0.1180410+00	0.2467700+00
21	-0.8231690-04	-0.5491400-03	-0.8606840-02	-0.4760370-01	-0.8320520-01
22	-0.2736520-03	0.3242650-03	-0.7639030-04	0.1101330-01	-0.1522580-01
23	0.3932520-04	0.1060390-02	-0.6016850-03	0.1119320-01	-0.2464590-01
24	0.3040020-03	0.6355410-03	0.2033350-02	-0.6134680-02	0.1232430-01
25	-0.2530060-04	-0.3418220-03	0.5784860-04	0.1688270-02	-0.4796360-03
26	0.1896080-03	-0.3841300-03	0.2010480-03	-0.1452520-02	0.1315550-02
27	0.1037050-04	0.1181340-03	-0.3238200-03	0.5960130-03	-0.7085850-03

	21	22	23	24	25
21	0.1042090+00				
22	-0.6943470-02	0.1292650+00			
23	-0.1051880-01	-0.1123060+00	0.2837270+00		
24	0.6834260-02	-0.4079330-01	0.9177880-01	0.1043730+00	
25	0.1557170-02	-0.7597900-02	-0.1318270-02	-0.3751900-02	0.1801750+00
26	0.1117340-04	-0.7121470-03	0.2730780-02	0.4807150-03	-0.2270560+00
27	-0.2828100-04	-0.2879420-02	0.5445450-03	-0.4705770-03	-0.4662900-01

	26	27
26	0.4373110+00	
27	0.1339470+00	0.5456520-01

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.3201410+00				
2	0.1995550-01	0.4171950+00			
3	0.3380240-02	0.1052870-02	0.3731760+00		
4	0.5127540-02	0.3270740-02	0.3591050-02	0.3682230+00	
5	0.3930860-02	0.1677870-02	0.3197800-02	0.3584720-02	0.3771010+00
6	0.6707190-02	0.1834040-01	0.1063800-02	0.1009680-02	-0.7964790-03
7	0.6036540-02	0.1255950-01	0.8846030-03	-0.9770390-03	0.8033280-03
8	0.9478220-03	-0.1253320-02	-0.4693540-03	-0.1792580-03	0.3990770-04
9	0.3130890-01	-0.2961450-02	0.1082410-01	-0.1640330-02	-0.5616040-02
10	0.2411080-01	0.1468070-01	-0.1404670-02	-0.9553740-02	-0.8578120-02
11	0.3035780-01	-0.3093840-02	-0.9477260-02	-0.4152090-02	-0.9208040-02
12	0.3051420-01	-0.3462700-02	-0.9325980-02	-0.9780230-02	-0.4089090-02
13	0.3500960-01	-0.3607880-01	0.1109570-03	-0.3154390-03	0.6140670-02
14	0.3482380-01	-0.3628930-01	-0.1326930-03	0.6274110-02	-0.7207780-03
15	0.2897010-03	0.4528970-01	-0.1111370-02	0.2269000-02	-0.4018350-03
16	-0.6213480-04	-0.3776040-02	0.5854090-03	0.1291450-01	-0.1186540-01
17	0.6771690-03	-0.1124690-02	-0.1506950-01	0.2704910-03	0.1491050-01
18	0.5718090-03	0.1531640-02	0.1496580-01	-0.1656520-01	-0.6342270-03
19	-0.2791530-02	-0.5115360-01	-0.8075740-03	0.1565730-02	-0.9804640-03
20	0.1805680-02	0.5339820-01	0.5133280-03	0.1122630-02	-0.1194400-02
21	-0.5470070-03	0.1868230-02	0.9586580-03	-0.1113820-02	-0.6758240-03

	6	7	8	9	10
6	0.3608010+00				
7	0.5033590-02	0.3793190+00			
8	0.1728070-03	-0.2290390-02	0.6048110+00		
9	-0.4997400-02	-0.5852000-02	-0.5903360-02	0.4248790+00	
10	0.1160920-02	0.5413880-03	-0.1216900-02	0.4814240-01	0.2481110+00
11	-0.1240960-02	0.5372800-02	0.1559480-02	-0.1624730-01	0.3894520-01
12	0.6056890-02	-0.1128050-02	0.1029160-03	-0.2065940-01	0.3721270-01
13	0.1551980-02	-0.1115030-01	0.1450430-02	0.8105800-01	-0.7779720-02
14	-0.1250060-01	-0.2031500-02	-0.2701380-02	0.7084780-01	-0.7800610-02
15	0.1054500-03	0.4196010-02	0.1620550-01	-0.1662570-01	-0.7891530-03
16	0.6909340-02	-0.9270140-02	-0.1098650-01	-0.3309890-02	0.2880210-03
17	0.4691730-03	0.1693870-03	-0.7147840-04	0.2420710-02	0.6380340-01

Table 4b. Force Constant Matrix for Ethanol [C_2H_6O] at the 6-31G* HF Level of Calculation. (CONTINUED 2)

18	-0.2622980-05	-0.5829540-03	-0.4251630-03	0.7042310-03	-0.6341210-01
19	0.7889450-02	0.1408420-01	0.4230600-02	0.8253740-01	-0.1347030-02
20	-0.1483750-01	-0.4566180-02	0.6463610-02	-0.8305170-01	0.1071590-03
21	-0.4952680-03	0.3997920-03	-0.1344010-02	-0.5791620-02	-0.1470720-02
	11	12	13	14	15
11	0.2561750+00				
12	0.3623870-01	0.2513750+00			
13	-0.9373480-02	0.3244350-01	0.2902290+00		
14	0.3185230-01	-0.8748900-02	0.4767610-01	0.2837170+00	
15	0.3709250-02	0.5139440-03	0.4865990-02	-0.1544960-01	0.2037950+00
16	-0.6654930-01	0.6370740-01	-0.8237870-01	0.8599920-01	-0.3014890-01
17	-0.1981280-02	-0.6190800-01	0.2714520-03	-0.9975520-03	0.2742400-03
18	0.6330800-01	0.5834510-02	0.9649590-03	0.6554530-04	0.7431320-03
19	0.1787980-02	0.1319990-02	0.2382860-01	-0.6095470-01	0.4224720-02
20	-0.9719240-03	-0.5497070-03	0.5775860-01	-0.2437260-01	0.2381080-01
21	-0.4350850-03	-0.8767010-03	0.2463290-02	-0.2831940-02	0.9964760-03
	16	17	18	19	20
16	0.5215210+00				
17	-0.1034490+00	0.2035270+00			
18	-0.1029560+00	-0.9859590-01	0.2069710+00		
19	-0.1594680+00	0.2191820-02	0.4408370-02	0.2572850+00	
20	-0.1605130+00	0.4218000-02	0.2254020-02	-0.9757560-01	0.2585100+00
21	0.3496840-02	-0.2025040-02	0.8544680-03	-0.3310950-02	0.1084880-02
	21				
21	0.1033450-01				

Table 4c. Force Constant Matrix for Ethanol [C_2H_6O] at the 6-31G* MP2 Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.619272D+00				
2	0.590620D-02	0.613484D+00			
3	-0.144678D-02	-0.140053D-02	0.516085D+00		
4	-0.858047D-01	-0.395346D-03	0.117112D-01	0.541526D+00	
5	0.148361D-02	-0.952676D-01	0.101175D-02	-0.158961D-01	0.670703D+00
6	0.226087D-01	-0.706008D-03	-0.223325D+00	-0.534781D-01	0.167407D-01
7	-0.168676D-01	0.240687D-02	-0.109974D-01	-0.221114D+00	-0.173169D-01
8	0.610741D-03	0.503730D-02	-0.111563D-02	0.256461D-01	-0.959813D-01
9	-0.483573D-01	0.510693D-03	-0.161124D-01	-0.426404D-01	-0.206677D-01
10	-0.293531D+00	0.132294D-01	-0.908879D-01	0.123035D-02	-0.335044D-03
11	0.134192D-01	-0.530367D-01	0.557131D-02	-0.306576D-04	-0.171632D-02
12	-0.898403D-01	0.557109D-02	-0.872310D-01	-0.344123D-01	0.205746D-02
13	-0.101247D+00	0.953265D-01	0.397917D-01	-0.163288D-02	0.763592D-03
14	0.961997D-01	-0.246676D+00	-0.777075D-01	0.135092D-03	0.144463D-02
15	0.387548D-01	-0.778473D-01	-0.830526D-01	0.173725D-01	-0.338396D-01
16	-0.129773D+00	-0.115039D+00	0.498907D-01	-0.134423D-02	-0.612704D-03
17	-0.115023D+00	-0.228655D+00	0.734863D-01	0.259375D-03	0.151845D-02
18	0.475180D-01	0.723499D-01	-0.809606D-01	0.216256D-01	0.310830D-01
19	0.334977D-02	-0.910474D-03	0.926122D-03	-0.114066D+00	-0.932733D-01
20	0.723567D-03	0.168712D-02	-0.224669D-02	-0.965011D-01	-0.220959D+00
21	0.179201D-01	0.297796D-01	-0.136574D-01	0.482890D-01	0.730042D-01
22	0.227765D-02	-0.867401D-04	0.577229D-03	-0.929899D-01	0.838393D-01
23	-0.139156D-02	0.270988D-02	0.175784D-02	0.941274D-01	-0.257544D+00
24	0.142768D-01	-0.310991D-01	-0.133966D-01	0.444376D-01	-0.843783D-01
25	0.232184D-02	-0.437768D-03	0.435012D-03	-0.258056D-01	0.413471D-01
26	-0.192808D-02	0.716028D-03	0.642970D-03	-0.734513D-02	-0.219881D-02
27	-0.143372D-02	0.284159D-02	0.164941D-02	-0.129046D-01	0.149891D-01

	6	7	8	9	10
6	0.525630D+00				
7	-0.706754D-01	0.413221D+00			
8	-0.259159D-02	-0.177891D+00	0.448013D+00		
9	-0.937172D-01	0.494470D-01	0.146963D+00	0.157962D+00	
10	0.263143D-02	0.149213D-02	0.372839D-03	-0.108081D-02	0.315767D+00
11	0.701907D-04	-0.276319D-03	0.172612D-02	-0.212195D-03	-0.148035D-01
12	-0.447948D-02	-0.312751D-02	0.147740D-03	-0.100244D-01	0.100806D+00
13	-0.128227D-02	0.155585D-02	-0.154423D-02	0.173809D-03	-0.116797D-01
14	0.185162D-02	-0.207197D-02	0.102254D-02	0.161913D-03	-0.110321D-02
15	-0.137112D-01	0.116074D-02	0.150683D-02	0.387611D-02	-0.490550D-02
16	-0.102201D-02	0.141085D-02	0.874040D-03	-0.344521D-05	-0.139310D-01
17	-0.115588D-02	0.132811D-02	0.142258D-03	-0.504205D-03	0.318944D-02
18	-0.141318D-01	0.498511D-04	-0.204264D-02	0.461576D-02	-0.621391D-02
19	0.489543D-01	-0.357511D-01	-0.250835D-01	0.179777D-02	0.157623D-03
20	0.721190D-01	-0.136307D-02	0.888121D-02	-0.285229D-02	0.558778D-05
21	-0.897899D-01	-0.144386D-01	-0.125454D-01	0.699219D-02	-0.539187D-03
22	0.396687D-01	-0.269697D-01	0.331904D-01	0.720777D-02	0.195057D-03
23	-0.817618D-01	0.200797D-02	0.288139D-02	0.141874D-02	-0.926501D-04
24	-0.888845D-01	-0.111038D-01	0.136086D-01	0.529500D-02	-0.428201D-03
25	0.125939D-01	-0.116977D+00	0.143825D+00	0.334553D-01	0.299026D-03
26	-0.456601D-02	0.193175D+00	-0.371723D+00	-0.124819D+00	-0.462721D-03
27	0.240796D-02	0.596853D-01	-0.143932D+00	-0.588860D-01	0.617245D-03

	11	12	13	14	15
11	0.506662D-01				
12	-0.525896D-02	0.907787D-01			
13	0.276165D-01	0.123311D-01	0.103648D+00		
14	-0.628176D-03	0.261321D-04	-0.106352D+00	0.262915D+00	
15	0.118794D-01	0.444165D-02	-0.438262D-01	0.866228D-01	0.906262D-01
16	-0.253269D-01	0.119019D-01	0.859262D-02	0.133216D-01	-0.614016D-02
17	0.312801D-02	-0.191192D-02	-0.158840D-01	-0.203459D-01	0.100417D-01
18	-0.115019D-01	0.424904D-02	-0.728515D-02	-0.965566D-02	0.386824D-02
19	-0.634454D-04	0.107008D-02	-0.411626D-03	-0.326991D-03	-0.521930D-03
20	-0.219357D-03	0.650764D-03	0.941426D-04	0.877862D-03	0.460622D-03
21	-0.103331D-03	0.122659D-02	0.144072D-03	-0.554652D-03	0.199840D-02

Table 4c. Force Constant Matrix for Ethanol [C_2H_6O] at the 6-31G* MP2 Level of Calculation. (CONTINUED 1)

22	-0.1017390-03	0.4640350-03	0.9533410-03	0.3606440-03	-0.5114720-03
23	-0.9417480-04	-0.6655780-03	-0.4945800-03	0.1727220-02	0.6712360-03
24	0.1913380-03	0.1364070-02	-0.4327750-04	0.4837470-03	-0.7406170-02
25	-0.4332120-03	0.8071120-03	0.2217620-03	-0.1624270-03	-0.1382810-02
26	0.1746720-03	-0.6166570-03	0.4747470-03	-0.3368100-03	0.5038070-03
27	-0.6357520-03	-0.3241750-03	-0.4123800-05	-0.1228580-02	-0.6402290-03

	16	17	18	19	20
16	0.1344750+00				
17	0.1262070+00	0.2421440+00			
18	-0.5476200-01	-0.7996230-01	0.8833970-01		
19	0.9476770-03	-0.2434170-03	-0.5814550-03	0.1349720+00	
20	0.4049260-03	0.1664980-02	-0.2823820-03	0.1112280+00	0.2283020+00
21	-0.4169140-04	-0.4328830-03	-0.7608170-02	-0.4675610-01	-0.7873750-01
22	-0.3680660-03	0.4283800-03	-0.2926090-03	0.9205130-02	-0.1462960-01
23	-0.7949900-04	0.8040390-03	-0.2316630-03	0.1066330-01	-0.2134320-01
24	0.1413480-03	0.2763150-03	0.1886250-02	-0.4861910-02	0.1177980-01
25	-0.9703320-05	-0.2622400-03	-0.5819290-04	0.1597030-02	0.3753340-04
26	0.2491180-03	-0.4000080-03	0.2441640-03	-0.1990740-02	0.1109680-02
27	0.3520930-04	0.1630170-03	-0.2581380-03	-0.2699280-04	-0.8913510-03

	21	22	23	24	25
21	0.9557750-01				
22	-0.5932970-02	0.1148950+00			
23	-0.1012570-01	-0.1035610+00	0.2683190+00		
24	0.5560890-02	-0.3890920-01	0.8840730-01	0.9581760-01	
25	0.1355380-02	-0.7198340-02	-0.1178470-02	-0.3509360-02	0.1455510+00
26	-0.2836230-03	0.5614000-03	0.2540280-02	0.7297510-03	-0.1827340+00
27	-0.2997090-03	-0.2271920-02	0.5294580-03	-0.2361990-03	-0.4369580-01

	26	27
26	0.3701180+00	
27	0.1281640+00	0.5658670-01

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.3084590+00				
2	0.1866350-01	0.3614270+00			
3	0.3247750-02	0.7533560-03	0.3551320+00		
4	0.4609850-02	0.2420730-02	0.1202340-02	0.3521600+00	
5	0.3538260-02	0.7898680-03	0.9418610-03	0.1269550-02	0.3600640+00
6	0.5689060-02	0.1506080-01	0.4961520-03	0.4471670-03	-0.7264100-03
7	0.4973290-02	0.9794840-02	0.3892400-03	-0.9239420-03	0.3293670-03
8	0.8706050-03	-0.3512530-02	-0.6766290-03	-0.3100810-03	0.7449850-04
9	0.2932230-01	-0.2396070-02	0.1043450-01	-0.1819700-02	-0.5857110-02
10	0.2452580-01	0.1285080-01	-0.1961550-02	-0.8888450-02	-0.7954190-02
11	0.3152450-01	-0.4158670-02	-0.8854920-02	-0.4317190-02	-0.8374900-02
12	0.3136640-01	-0.4203180-02	-0.8780360-02	-0.8940590-02	-0.3922680-02
13	0.3558660-01	-0.3290020-01	-0.2608390-03	-0.7562180-03	0.5529430-02
14	0.3483380-01	-0.3313120-01	-0.4810990-03	0.5568320-02	-0.1036190-02
15	-0.4474030-03	0.5221120-01	-0.1026310-02	0.2364330-02	-0.2097400-03
16	0.3974310-04	-0.4914480-02	0.6557320-03	0.1242190-01	-0.1143560-01
17	0.1128870-02	-0.8079030-03	-0.1442370-01	0.5247360-03	0.1436840-01
18	0.3396150-03	0.1191200-02	0.1424900-01	-0.1590880-01	-0.9602630-03
19	-0.2991610-02	-0.4676370-01	-0.5838820-03	0.1400370-02	-0.9629210-03
20	0.1749270-02	0.4994980-01	0.3291660-03	0.1168630-02	-0.1002500-02
21	0.1125000-03	0.2030210-02	0.8911260-03	-0.1139150-02	-0.6649490-03

	6	7	8	9	10
6	0.3368240+00				
7	0.2653110-02	0.3562030+00			
8	-0.4322900-03	-0.1841230-02	0.5111930+00		
9	-0.3847600-02	-0.5495830-02	-0.6586670-02	0.3839750+00	
10	0.1022640-02	0.2978720-03	-0.1615410-02	0.4325520-01	0.2232630+00
11	-0.1720810-02	0.4748000-02	0.2112570-02	-0.1415040-01	0.3504950-01
12	0.5235160-02	-0.1546010-02	0.2889570-03	-0.1897300-01	0.3307070-01
13	0.2642180-02	-0.1091430-01	0.2379860-02	0.7076100-01	-0.6917920-02
14	-0.1216100-01	-0.2065090-02	-0.3174350-02	0.6038790-01	-0.6745260-02
15	-0.3070360-04	0.3485900-02	0.1859190-01	-0.1654610-01	-0.6232860-03
16	0.4370700-02	-0.8587610-02	-0.1241020-01	-0.3494260-02	0.2207530-03
17	0.2699260-03	0.1713000-03	0.2714830-04	0.3469170-02	0.5876910-01

Table 4c. Force Constant Matrix for Ethanol [C_2H_6O] at the 6-31G* MP2 Level of Calculation. (CONTINUED 2)

18	0.6971640-04	-0.4061730-03	-0.5557740-03	-0.4974950-04	-0.5846990-01
19	0.9842780-02	0.1354110-01	0.4581550-02	0.7406270-01	-0.1757680-02
20	-0.1392080-01	-0.4925340-02	0.7573600-02	-0.7492550-01	0.2202830-03
21	-0.1023510-02	0.3058580-03	-0.1428190-02	-0.4779480-02	-0.1706710-02
	11	12	13	14	15
11	0.2337050+00				
12	0.3133870-01	0.2290020+00			
13	-0.8146870-02	0.2924750-01	0.2630150+00		
14	0.2862820-01	-0.7343880-02	0.4343980-01	0.2559140+00	
15	0.3561100-02	0.6028510-03	0.3728870-02	-0.1422360-01	0.1933980+00
16	-0.6155160-01	0.5883540-01	-0.7160830-01	0.7562820-01	-0.2684130-01
17	-0.1601030-02	-0.5683390-01	0.3062660-03	-0.8929600-03	0.3362070-03
18	0.5827970-01	0.6115760-02	0.8281350-03	0.1620880-03	0.7000070-03
19	0.1875570-02	0.2091190-02	0.1771150-01	-0.5617690-01	0.2584620-02
20	-0.1568480-02	-0.7997810-03	0.5310290-01	-0.1876000-01	0.2212850-01
21	-0.2378110-03	-0.6748340-03	0.3025970-02	-0.2766840-02	0.1579310-02
	16	17	18	19	20
16	0.4720920+00				
17	-0.9523530-01	0.1886580+00			
18	-0.9474350-01	-0.9113230-01	0.1921490+00		
19	-0.1422050+00	0.2614780-02	0.4124090-02	0.2311570+00	
20	-0.1451780+00	0.3943730-02	0.2685050-02	-0.8865860-01	0.2343060+00
21	0.4439530-02	-0.2118650-02	0.9972920-03	-0.3409280-02	0.4007340-03
	21				
21	0.1141650-01				

Table 4d. Force Constant Scaling Constants, Q(I), and C matrix for Ethanol [C_2H_6O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation.

Q Values

I	Q(I)
1	0.963508E+00
2	0.866325E+00
3	0.951649E+00
4	0.956379E+00
5	0.954820E+00
6	0.933547E+00
7	0.939058E+00
8	0.845211E+00
9	0.903729E+00
10	0.899851E+00
11	0.912287E+00
12	0.910999E+00
13	0.906231E+00
14	0.902007E+00
15	0.948980E+00
16	0.905222E+00
17	0.926943E+00
18	0.928386E+00
19	0.898448E+00
20	0.906370E+00
21	0.110469E+01

C Matrix (21,21)

		COLUMN 1	COLUMN 2	COLUMN 3
ROW	1	0.1000000000000+01		
ROW	2	0.102367492518D+01	0.1000000000000+01	
ROW	3	0.100338763036D+01	0.788036516635D+00	0.1000000000000+01
ROW	4	0.936558449491D+00	0.8130991859790+00	0.3509565753800+00
ROW	5	0.938456420812D+00	0.5176001549340+00	0.3089845663000+00
ROW	6	0.894343618097D+00	0.9131244815800+00	0.4948221633450+00
ROW	7	0.866127270089D+00	0.8646463120430+00	0.1000000000000+01
ROW	8	0.1000000000000+01	0.3275180811820+01	0.1000000000000+01
ROW	9	0.100365014789D+01	0.9143996207290+00	0.1039499679300+01
ROW	10	0.1092439534540+01	0.9914204588600+00	0.1512582069210+01
ROW	11	0.1107603468660+01	0.1511996282090+01	0.1002762087230+01
ROW	12	0.1097175789250+01	0.1366355026040+01	0.1011161658850+01
ROW	13	0.1087806136660+01	0.1029168098780+01	0.1000000000000+01
ROW	14	0.1072979108030+01	0.1032790400050+01	0.1000000000000+01
ROW	15	0.1000000000000+01	0.1271438455460+01	0.9717422035040+00
ROW	16	0.1000000000000+01	0.1469682091980+01	0.1000000000000+01
ROW	17	0.1000000000000+01	0.8016056414050+00	0.1019091743920+01
ROW	18	0.1000000000000+01	0.8672115232710+00	0.1012935375800+01
ROW	19	0.1151829576640+01	0.1036204943960+01	0.1000000000000+01
ROW	20	0.103665764488D+01	0.1055634444230+01	0.1000000000000+01
ROW	21	0.1000000000000+01	0.1110832481590+01	0.1000000000000+01

		COLUMN 4	COLUMN 5	COLUMN 6
ROW	4	0.1000000000000+01		
ROW	5	0.3706103968440+00	0.1000000000000+01	
ROW	6	0.4687090088720+00	0.1000000000000+01	0.1000000000000+01
ROW	7	0.1000000000000+01	0.1000000000000+01	0.5629423059530+00
ROW	8	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	9	0.1193257364780+01	0.1122724031210+01	0.8382220204210+00
ROW	10	0.100288669148D+01	0.1000363621250+01	0.9610912203750+00
ROW	11	0.1113149215970+01	0.9745086317910+00	0.1502588040970+01
ROW	12	0.9793612366660+00	0.1028577388770+01	0.9372457724540+00
ROW	13	0.1000000000000+01	0.9680211621530+00	0.1850928377500+01
ROW	14	0.955547926462D+00	0.1000000000000+01	0.1060137826020+01

Table 4d. Force Constant Scaling Constants, Q(I), and C matrix for Ethanol [C_2H_6O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED)

ROW	15	0.1093782060100+01	0.1000000000000+01	0.1000000000000+01
ROW	16	0.1033753079440+01	0.1036664972570+01	0.6881265746600+00
ROW	17	0.1000000000000+01	0.1024307998900+01	0.1000000000000+01
ROW	18	0.1019204105280+01	0.1000000000000+01	0.1000000000000+01
ROW	19	0.9648589340160+00	0.1000000000000+01	0.1362248585210+01
ROW	20	0.1118071977000+01	0.9022328859600+00	0.1019959623270+01
ROW	21	0.9950177483770+00	0.1000000000000+01	0.1000000000000+01

		COLUMN 7	COLUMN 8	COLUMN 9
ROW	7	0.1000000000000+01		
ROW	8	0.9023419338490+00	0.1000000000000+01	
ROW	9	0.1019443985600+01	0.1276628964550+01	0.1000000000000+01
ROW	10	0.1000000000000+01	0.1522165914240+01	0.9963370809920+00
ROW	11	0.9547692742250+00	0.1542709326850+01	0.9591857196520+00
ROW	12	0.1481756466220+01	0.1000000000000+01	0.1012137306810+01
ROW	13	0.1061071666820+01	0.1874791126200+01	0.9646274459050+00
ROW	14	0.1104516327250+01	0.1345805101890+01	0.9440610570330+00
ROW	15	0.8800403911150+00	0.1281001125600+01	0.1074648014430+01
ROW	16	0.1004759563450+01	0.1291392354840+01	0.1157197556700+01
ROW	17	0.1000000000000+01	0.1000000000000+01	0.1565805869740+01
ROW	18	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	19	0.1046712861170+01	0.1242743580060+01	0.9958256058520+00
ROW	20	0.1169185383310+01	0.1338724344510+01	0.9968030699180+00
ROW	21	0.1000000000000+01	0.1099709081600+01	0.8259245748960+00

		COLUMN 10	COLUMN 11	COLUMN 12
ROW	10	0.1000000000000+01		
ROW	11	0.9932926928560+00	0.1000000000000+01	
ROW	12	0.9815373010510+00	0.9486021410610+00	0.1000000000000+01
ROW	13	0.9847054390080+00	0.9558837696250+00	0.9921609466920+00
ROW	14	0.9597984408440+00	0.9907911562480+00	0.9259937009000+00
ROW	15	0.1000000000000+01	0.1031818353590+01	0.1000000000000+01
ROW	16	0.1000000000000+01	0.1017778168860+01	0.1016979334640+01
ROW	17	0.1008541124030+01	0.8787467331420+00	0.9990231126770+00
ROW	18	0.1008812344370+01	0.1000295964100+01	0.1139784597380+01
ROW	19	0.1451206300490+01	0.1158670240290+01	0.1751125320900+01
ROW	20	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	21	0.1163922454320+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 13	COLUMN 14	COLUMN 15
ROW	13	0.1000000000000+01		
ROW	14	0.1007772511980+01	0.1000000000000+01	
ROW	15	0.8263384182900+00	0.9950790623780+00	0.1000000000000+01
ROW	16	0.9597347548290+00	0.9732104303930+00	0.9605651629280+00
ROW	17	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	18	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	19	0.8237440359630+00	0.1023762990800+01	0.6625592421950+00
ROW	20	0.1014446014610+01	0.8512826858400+00	0.1002065903190+01
ROW	21	0.1227745166560+01	0.9787539610320+00	0.1000000000000+01

		COLUMN 16	COLUMN 17	COLUMN 18
ROW	16	0.1000000000000+01		
ROW	17	0.1005000797610+01	0.1000000000000+01	
ROW	18	0.1003816285290+01	0.9963758978160+00	0.1000000000000+01
ROW	19	0.9888184653010+00	0.1307244664510+01	0.1024329006630+01
ROW	20	0.9985259538120+00	0.1020051993480+01	0.1298610522550+01
ROW	21	0.1269585214320+01	0.1033899932990+01	0.1000000000000+01

		COLUMN 19	COLUMN 20	COLUMN 21
ROW	19	0.1000000000000+01		
ROW	20	0.1006885642580+01	0.1000000000000+01	
ROW	21	0.1033573699740+01	0.3691498624800+00	0.1000000000000+01

Table 5a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Isopropanol [C_3H_8O] Based on Several Levels of Calculation.

H8

H4 O7 H10

H5 C1 C2 C3 H11

H6 H9 H12

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
geometry					
$r(C_1-C_2)$/A	1.5315	1.5406	1.5248	1.5203	-
$r(C_2-C_3)$/A	1.5250	1.5339	1.5191	1.5143	-
$r(C_1-H_4)$/A	1.0831	1.0941	1.0852	1.0931	-
$r(C_1-H_5)$/A	1.0860	1.0969	1.0874	1.0953	-
$r(C_1-H_6)$/A	1.0834	1.0945	1.0856	1.0940	-
$r(C_2-O_7)$/A	1.4477	1.4776	1.4094	1.4323	-
$r(O_7-H_8)$/A	0.9666	0.9935	0.9472	0.9725	-
$r(C_2-H_9)$/A	1.0855	1.1000	1.0896	1.1013	-
$r(C_3-H_{10})$/A	1.0835	1.0943	1.0854	1.0933	-
$r(C_3-H_{11})$/A	1.0821	1.0932	1.0839	1.0919	-
$r(C_3-H_{12})$/A	1.0828	1.0939	1.0851	1.0931	-
$\phi(C_3-C_2-C_1)$/°	111.9616	112.0946	112.4207	112.4301	-
$\phi(H_4-C_1-C_2)$/°	109.2445	108.6746	110.2846	109.5537	-
$\phi(H_5-C_1-C_2)$/°	111.0025	110.7839	110.9593	110.9746	-
$\phi(H_6-C_1-C_2)$/°	110.8077	110.7710	111.1378	111.2094	-
$\phi(O_7-C_2-C_1)$/°	110.4079	110.4407	110.9442	110.3316	-
$\phi(H_8-O_7-C_2)$/°	110.5621	107.0323	109.5731	107.3316	-
$\phi(H_9-C_2-C_1)$/°	109.5652	109.4560	108.8290	109.1527	-
$\phi(H_{10}-C_3-C_2)$/°	110.8800	110.6701	110.8761	110.8277	-
$\phi(H_{11}-C_3-C_2)$/°	109.7385	109.5732	110.2293	110.1473	-
$\phi(H_{12}-C_3-C_2)$/°	109.2014	108.7706	110.2006	109.5848	-

Table 5a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Isopropanol [C_3H_8O] Based on Several Levels of Calculation. (CONTINUED 1)

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
$\tau(H_4\text{-}C_1\text{-}C_2\text{-}C_3)$/°	60.0026	59.8880	59.5285	59.3134	-
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$/°	179.5356	179.3000	179.2300	178.8883	-
$\tau(H_6\text{-}C_1\text{-}C_2\text{-}C_3)$/°	-60.2605	-60.3374	-61.0162	-61.1097	-
$\tau(O_7\text{-}C_2\text{-}C_1\text{-}H_4)$/°	-56.7231	-56.0466	-59.6497	-58.7119	-
$\tau(H_8\text{-}O_7\text{-}C_2\text{-}C_1)$/°	-60.0627	-59.4913	-60.1592	-58.4592	-
$\tau(H_9\text{-}C_2\text{-}C_1\text{-}H_4)$/°	-178.2449	-178.3750	-180.0100	-179.5829	-
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$/°	61.4332	61.5601	60.4121	61.0232	-
$\tau(H_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$/°	-182.2363	182.4715	180.7291	181.6038	-
$\tau(H_{12}\text{-}C_3\text{-}C_2\text{-}C_1)$/°	-59.1097	-58.8520	-59.8985	-59.1881	-
E/a.u.	-192.048260	-192.046084	-193.115416	-193.706552	-
frequencies (cm^{-1})					
$\tilde{\nu}_1$	235	234	241	240	
$\tilde{\nu}_2$	279	275	287	289	
$\tilde{\nu}_3$	325	334	328	331	
$\tilde{\nu}_4$	388	366	387	372	
$\tilde{\nu}_5$	420	395	446	425	
$\tilde{\nu}_6$	497	469	520	496	
$\tilde{\nu}_7$	858	818	884	856	
$\tilde{\nu}_8$	1020	958	1013	960	
$\tilde{\nu}_9$	1039	972	1030	986	
$\tilde{\nu}_{10}$	1051	1003	1074	1008	
$\tilde{\nu}_{11}$	1168	1117	1178	1131	
$\tilde{\nu}_{12}$	1265	1180	1273	1201	
$\tilde{\nu}_{13}$	1305	1239	1308	1236	
$\tilde{\nu}_{14}$	1387	1325	1401	1319	
$\tilde{\nu}_{15}$	1511	1435	1518	1426	

Table 5a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Isopropanol [C_3H_8O] Based on Several Levels of Calculation. (CONTINUED 2)

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
$\tilde{\nu}_{16}$	1548	1474	1540	1444	
ν_{17}	1563	1479	1568	1470	
ν_{18}	1580	1496	1585	1490	
ν_{19}	1652	1585	1628	1547	
ν_{20}	1660	1592	1633	1551	
ν_{21}	1666	1598	1643	1562	
ν_{22}	1682	1612	1654	1573	
ν_{23}	3184	3044	3166	3051	
ν_{24}	3194	3079	3196	3099	
ν_{25}	3210	3096	3212	3114	
ν_{26}	3250	3150	3254	3184	
ν_{27}	3271	3172	3271	3203	
ν_{28}	3279	3178	3280	3209	
ν_{29}	3284	3181	3288	3215	
ν_{30}	3860	3498	4106	3762	

Table 5b. Force Constant Matrix for Isopropanol [C_3H_8O] at the 6-31G* HF Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.650431D+00				
2	0.172972D-02	0.661637D+00			
3	-0.995722D-03	-0.357056D-03	0.555728D+00		
4	-0.100370D+00	0.288889D-02	0.693484D-04	0.636495D+00	
5	0.554982D-02	-0.958095D-01	-0.849444D-02	-0.501626D-01	0.641763D+00
6	-0.687152D-02	-0.204843D-01	-0.228362D+00	0.309898D-02	0.305706D-01
7	0.224167D-02	0.175881D-02	-0.538302D-02	-0.215049D+00	0.550594D-02
8	-0.265547D-03	0.237942D-02	-0.173052D-02	0.213307D-01	-0.947951D-01
9	-0.400311D-01	0.326745D-03	-0.170629D-01	-0.565173D-01	-0.248357D-02
10	-0.125525D+00	0.111189D+00	0.464698D-01	0.115073D-03	-0.586290D-04
11	0.111059D+00	-0.248200D+00	-0.800440D-01	-0.229141D-03	-0.193172D-02
12	0.455925D-01	-0.765398D-01	-0.912324D-01	0.198370D-01	-0.363643D-01
13	-0.304774D+00	-0.281987D-02	-0.913516D-01	-0.453789D-04	-0.131611D-02
14	-0.234242D-02	-0.595816D-01	-0.165593D-02	-0.136406D-02	-0.135766D-02
15	-0.891896D-01	-0.871349D-03	-0.935863D-01	-0.414669D-01	-0.449290D-03
16	-0.117242D+00	-0.105828D+00	0.470158D-01	-0.147541D-02	0.599149D-03
17	-0.105207D+00	-0.249918D+00	0.835027D-01	0.132014D-02	0.158545D-03
18	0.449786D-01	0.802180D-01	-0.976938D-01	0.175914D-01	0.327890D-01
19	-0.309151D-02	-0.104454D-01	0.418029D-02	-0.140473D+00	-0.765061D-01
20	-0.123971D-01	-0.134127D-01	0.929287D-02	-0.361691D-01	-0.221254D+00
21	0.261216D-01	0.490325D-01	-0.167197D-01	0.688425D-03	0.560346D-01
22	0.158240D-02	0.192558D-02	0.343366D-03	-0.197514D-01	0.522553D-02
23	0.217307D-03	0.115496D-02	-0.332084D-03	-0.437507D-01	-0.761389D-03
24	0.287704D-02	-0.136638D-03	0.117216D-02	0.199549D-01	0.142046D-02
25	0.209742D-02	0.284704D-03	-0.182943D-02	-0.135084D+00	0.107936D+00
26	0.190780D-02	0.192907D-02	-0.531707D-03	0.104342D+00	-0.223172D+00
27	0.209783D-01	-0.326287D-01	-0.139295D-01	0.455254D-01	-0.742537D-01
28	0.101178D-02	-0.302883D-03	0.794050D-03	-0.898945D-02	-0.301397D-01
29	-0.984345D-04	-0.458793D-03	0.466917D-03	0.313329D-02	-0.135077D-03
30	0.433664D-03	-0.170208D-03	0.170493D-04	-0.446716D-02	-0.133671D-01
31	-0.771292D-02	-0.453027D-03	-0.107518D-02	0.333148D-02	-0.109840D-03
32	0.778185D-04	0.230365D-03	-0.639830D-04	-0.262273D-03	-0.110953D-02
33	-0.397255D-02	0.316988D-03	0.584509D-03	0.374452D-02	0.587035D-03
34	0.135115D-02	0.725043D-04	0.176233D-02	-0.187043D-01	0.334762D-01
35	-0.231076D-03	0.505500D-04	-0.527387D-04	-0.107672D-02	-0.159567D-02
36	0.786605D-04	0.129384D-02	0.108486D-02	-0.805851D-02	0.140107D-01

	6	7	8	9	10
6	0.588411D+00				
7	-0.485485D-01	0.579156D+00			
8	0.385792D-02	0.452957D-02	0.661260D+00		
9	-0.119709D+00	-0.343495D-01	-0.303374D-02	0.650884D+00	
10	-0.226818D-03	0.493543D-03	-0.114214D-02	-0.295621D-03	0.129280D+00
11	0.138309D-02	0.160950D-05	0.351804D-04	0.254556D-03	-0.124030D+00
12	-0.131841D-01	0.147533D-02	-0.541309D-03	0.198925D-02	-0.500239D-01
13	0.347059D-02	0.134760D-02	-0.485647D-03	-0.589374D-03	-0.158206D-01
14	0.313391D-03	0.152235D-03	0.305382D-03	-0.360837D-04	0.292934D-01
15	-0.111641D-01	0.286022D-02	0.162372D-03	-0.830192D-02	0.126977D-01
16	-0.117248D-02	-0.253915D-03	0.718380D-04	-0.103872D-03	0.103607D-01
17	-0.276293D-02	-0.483010D-03	-0.430161D-03	-0.125471D-03	-0.146041D-01
18	-0.307726D-02	0.258788D-03	0.382338D-03	0.149025D-02	-0.795480D-02
19	0.292833D-01	-0.289422D-01	-0.482822D-01	0.175575D-01	-0.205015D-03
20	0.739102D-01	-0.862192D-02	-0.657098D-02	0.384300D-02	-0.826970D-03
21	-0.113550D+00	-0.676607D-02	-0.117340D-01	0.723596D-02	-0.433600D-03
22	-0.101642D-01	-0.299854D-03	-0.503730D-02	0.250593D-02	-0.274404D-03
23	-0.146107D-01	-0.266854D-02	-0.675626D-02	0.308494D-02	0.557374D-03
24	0.506425D-02	0.128239D-02	0.197153D-02	-0.992427D-03	0.121253D-03
25	0.437643D-01	-0.180058D-01	0.302441D-01	0.127367D-01	0.113513D-02
26	-0.730290D-01	0.274794D-03	0.207266D-02	-0.489871D-03	-0.310346D-03
27	-0.978221D-01	-0.895338D-02	0.123068D-01	0.596335D-02	-0.191401D-03
28	0.147692D-01	-0.132595D+00	-0.113544D+00	0.391877D-01	-0.635814D-05
29	0.196590D-04	-0.117107D+00	-0.248317D+00	0.672719D-01	-0.732255D-04
30	0.370335D-02	0.417694D-01	0.692092D-01	-0.846423D-01	-0.437197D-04

Table 5b. Force Constant Matrix for Isopropanol [C_3H_8O] at the 6-31G* HF Level of Calculation. (CONTINUED 1)

31	-0.399751D-01	-0.602950D-01	-0.165255D-04	0.170446D-01	0.517440D-04
32	0.110828D-02	0.630112D-03	-0.597088D-01	0.309065D-02	-0.344929D-04
33	-0.150328D-01	0.121432D-01	0.242586D-02	-0.349212D+00	0.123900D-03
34	0.125723D-01	-0.127798D+00	0.112597D+00	0.428542D-01	0.395530D-03
35	-0.276228D-03	0.116028D+00	-0.249475D+00	-0.717030D-01	0.406999D-04
36	0.472249D-02	0.442111D-01	-0.732763D-01	-0.876422D-01	-0.242809D-03
	11	12	13	14	15
11	0.265412D+00				
12	0.876414D-01	0.963636D-01			
13	-0.792630D-03	-0.546681D-02	0.330342D+00		
14	0.260107D-02	0.119280D-01	0.377965D-02	0.554651D-01	
15	0.178296D-02	0.488323D-02	0.100939D+00	0.142299D-02	0.983814D-01
16	0.150870D-01	-0.859851D-02	-0.150989D-01	-0.295718D-01	0.136445D-01
17	-0.225365D-01	0.109970D-01	0.153888D-04	0.129722D-02	-0.145000D-02
18	-0.104150D-01	0.523109D-02	-0.520116D-02	-0.122847D-01	0.543091D-02
19	0.186085D-03	-0.159355D-02	0.264035D-02	0.779725D-03	0.969095D-03
20	0.267222D-02	0.157984D-02	0.177160D-02	0.208104D-04	-0.141952D-02
21	-0.300770D-03	0.461501D-02	-0.118766D-03	-0.397949D-03	0.403957D-02
22	-0.103643D-03	0.144104D-03	0.102458D-03	-0.136783D-03	0.895418D-03
23	-0.176578D-03	-0.169143D-03	0.356954D-03	0.212866D-03	0.107828D-02
24	-0.822494D-04	-0.332805D-03	-0.927661D-03	0.696979D-03	-0.103367D-02
25	-0.425421D-03	-0.121097D-03	0.915585D-03	-0.487055D-03	0.880084D-03
26	0.146472D-02	0.318631D-03	-0.453977D-03	-0.921591D-04	-0.243869D-03
27	0.560587D-04	-0.850046D-02	-0.103893D-02	0.159897D-03	0.191393D-02
28	0.716692D-04	-0.107817D-03	0.150462D-03	0.419332D-03	0.170175D-03
29	-0.396365D-05	0.579136D-04	0.130563D-03	0.254453D-03	-0.325438D-03
30	-0.778169D-04	-0.159064D-04	0.178037D-03	0.461008D-04	0.291994D-03
31	-0.277189D-03	0.104348D-04	-0.562278D-04	-0.777264D-04	-0.247500D-02
32	0.277267D-03	0.454626D-03	-0.115737D-04	0.593470D-03	0.640545D-04
33	0.625966D-04	0.355673D-03	-0.152645D-03	-0.422781D-04	-0.100678D-02
34	-0.547105D-03	-0.114766D-02	0.296134D-03	-0.444460D-03	0.757441D-04
35	0.386729D-03	0.637204D-03	-0.174360D-03	0.281054D-03	0.248800D-03
36	-0.260808D-03	-0.172168D-03	0.259819D-03	-0.150433D-03	0.151741D-03
	16	17	18	19	20
16	0.121308D+00				
17	0.118470D+00	0.268146D+00			
18	-0.503633D-01	-0.917524D-01	0.993142D-01		
19	0.168461D-02	-0.406013D-03	0.208813D-02	0.692130D+00	
20	0.116887D-03	0.192123D-02	0.376665D-02	0.112835D+00	0.320083D+00
21	0.515001D-03	0.105875D-02	-0.117055D-01	0.150778D+00	-0.125169D+00
22	0.518420D-03	0.193005D-03	-0.811739D-03	-0.531911D+00	-0.296028D-01
23	0.345998D-03	-0.162618D-03	-0.468553D-03	0.199121D-01	-0.422623D-01
24	-0.751655D-03	-0.383807D-03	-0.172767D-04	-0.195763D+00	0.150051D-01
25	-0.106462D-03	0.765190D-04	0.217070D-03	0.117075D-01	-0.265689D-01
26	0.291033D-03	0.563231D-03	-0.147834D-02	0.222701D-02	-0.445076D-01
27	0.289016D-03	0.942241D-03	0.129471D-02	-0.602265D-02	0.200774D-01
28	0.161800D-03	0.400753D-03	-0.922619D-03	-0.100493D-01	-0.626714D-03
29	0.223049D-03	0.720055D-03	-0.341570D-03	-0.566536D-03	0.127800D-02
30	-0.606241D-03	-0.934903D-04	-0.459544D-03	-0.394511D-02	-0.412818D-03
31	0.104791D-03	0.308946D-03	0.205467D-03	0.290479D-02	0.105084D-02
32	0.101105D-03	0.228118D-03	-0.384358D-03	0.799964D-04	0.857194D-04
33	0.160634D-03	0.192843D-04	0.262365D-03	0.860738D-03	-0.368793D-03
34	0.383113D-04	-0.846767D-04	-0.858382D-04	0.360389D-02	-0.960779D-03
35	0.934987D-04	0.134880D-04	-0.311451D-04	0.186419D-03	0.194729D-02
36	-0.289554D-04	0.481697D-04	-0.702222D-04	0.160712D-02	-0.105312D-03
	21	22	23	24	25
21	0.197162D+00				
22	-0.165198D+00	0.548082D+00			
23	0.317902D-01	0.261524D-01	0.476445D-01		
24	-0.809051D-01	0.173323D+00	-0.187439D-01	0.762423D-01	
25	-0.354641D-02	0.198229D-02	0.470171D-03	-0.580133D-03	0.139567D+00
26	0.573317D-03	0.109114D-02	0.480807D-03	-0.550618D-04	-0.110125D+00
27	0.784259D-02	-0.545329D-03	-0.127644D-02	-0.108635D-03	-0.483632D-01
28	-0.377310D-02	-0.800036D-03	-0.205480D-02	0.555403D-03	0.962738D-03
29	-0.267224D-03	0.142689D-03	0.483927D-03	0.254128D-03	-0.787643D-03
30	-0.302934D-03	-0.623599D-03	-0.625782D-03	0.826134D-03	0.704561D-03

Table 5b. Force Constant Matrix for Isopropanol [C_3H_8O] at the 6-31G* HF Level of Calculation. (CONTINUED 2)

31	0.153144D-02	0.256976D-03	0.403438D-03	0.275564D-05	0.181640D-02
32	-0.656325D-03	0.898000D-04	-0.576624D-04	0.927034D-04	-0.392729D-03
33	0.224245D-02	0.250729D-05	-0.371697D-06	0.205660D-03	-0.372238D-03
34	0.201545D-03	0.512052D-03	0.582836D-04	-0.937529D-04	-0.698751D-02
35	0.354960D-04	0.604011D-04	0.199715D-03	-0.393038D-04	-0.225192D-03
36	0.449522D-04	0.129302D-03	0.273457D-03	-0.120520D-03	-0.349032D-02

	26	27	28	29	30
26	0.259257D+00				
27	0.741180D-01	0.102494D+00			
28	0.110882D-02	0.779246D-03	0.139037D+00		
29	0.680825D-03	-0.402426D-03	0.129378D+00	0.266768D+00	
30	0.205069D-03	0.273727D-03	-0.447572D-01	-0.767608D-01	0.844308D-01
31	0.201317D-03	0.894348D-03	-0.731031D-03	0.155980D-02	0.192737D-01
32	-0.933179D-04	0.472948D-03	0.112922D-03	0.149561D-02	0.318062D-01
33	0.517960D-03	0.962282D-03	0.793445D-03	0.458639D-03	-0.785500D-02
34	-0.554233D-03	-0.335150D-02	0.118475D-01	-0.159339D-01	-0.791634D-02
35	0.141646D-02	0.428088D-03	0.151771D-01	-0.227669D-01	-0.975848D-02
36	0.949134D-04	-0.383909D-03	-0.748849D-02	0.956830D-02	0.373267D-02

	31	32	33	34	35
31	0.609956D-01				
32	-0.870764D-03	0.557787D-01			
33	-0.140954D-01	-0.395726D-02	0.377830D+00		
34	-0.666597D-03	0.480080D-03	0.763843D-03	0.136112D+00	
35	-0.171927D-02	0.228005D-02	-0.196593D-04	-0.128159D+00	0.267262D+00
36	0.186579D-01	-0.320275D-01	-0.933669D-02	-0.456348D-01	0.805310D-01

	36
36	0.879890D-01

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.315853D+00				
2	0.112704D-01	0.329170D+00			
3	0.388346D-02	0.536626D-03	0.375307D+00		
4	0.438779D-02	-0.390774D-03	0.352276D-02	0.368149D+00	
5	0.260309D-02	-0.522400D-05	0.313101D-02	0.362560D-02	0.373977D+00
6	0.208408D-01	0.179291D-01	0.158079D-02	0.296058D-02	0.113429D-02
7	0.476320D-03	-0.881066D-03	0.562818D-05	0.174372D-04	-0.447138D-03
8	0.737300D-02	0.664684D-02	-0.713754D-03	0.106778D-02	0.108744D-02
9	0.100631D-03	0.265763D-02	-0.677681D-04	-0.326701D-04	0.108330D-02
10	-0.322167D-03	0.341987D-02	-0.119494D-03	0.467153D-03	-0.193056D-04
11	0.651389D-03	0.427195D-02	0.883290D-03	-0.116200D-03	-0.783833D-04
12	0.434477D-01	0.561565D-03	-0.323973D-02	0.834758D-02	-0.273451D-02
13	0.303869D-01	-0.267058D-02	-0.450221D-02	-0.968385D-02	-0.936873D-02
14	0.297943D-01	0.646402D-02	-0.916643D-02	-0.490355D-02	-0.951099D-02
15	0.249511D-01	0.847927D-04	-0.869171D-02	-0.962420D-02	-0.313163D-02
16	0.361343D-01	-0.242723D-01	-0.538487D-02	-0.177939D-02	0.113228D-01
17	0.502645D-03	0.572448D-02	-0.479924D-03	0.229848D-02	-0.104505D-02
18	0.366393D-01	-0.203920D-01	0.661565D-02	-0.133032D-03	0.177400D-03
19	0.194967D-03	0.264600D-01	0.450285D-04	-0.620873D-03	0.485126D-03
20	0.680824D-02	0.309056D-01	0.489009D-03	0.196068D-02	0.464039D-03
21	-0.254100D-02	0.313593D-01	0.153968D-02	-0.760099D-03	0.600373D-04
22	0.147948D-02	0.579130D-02	-0.316932D-02	-0.143137D-01	0.159264D-01
23	0.110349D-02	-0.845523D-04	0.148950D-01	-0.198255D-03	-0.149867D-01
24	-0.164030D-02	-0.358532D-03	-0.140942D-01	0.155981D-01	0.784468D-03
25	0.282779D-02	-0.335428D-01	0.285146D-02	-0.355355D-02	-0.671874D-04
26	-0.468034D-03	0.565304D-03	-0.777322D-03	-0.124980D-02	0.104369D-02
27	-0.334566D-02	0.272943D-01	-0.130397D-03	0.144862D-02	-0.100325D-02
28	0.348816D-03	0.383035D-03	0.394410D-04	-0.294799D-03	0.177527D-04
29	0.170700D-03	0.220632D-03	0.770050D-03	0.349564D-04	-0.709596D-03
30	0.572035D-03	-0.907976D-03	-0.819118D-04	0.332586D-03	-0.302906D-04

	6	7	8	9	10
6	0.403754D+00				
7	-0.169475D-02	0.605423D+00			
8	0.186043D-01	0.166655D-03	0.355602D+00		
9	0.110105D-02	0.327329D-04	0.102761D-02	0.374390D+00	
10	0.865408D-03	-0.567185D-04	0.923858D-03	0.332833D-02	0.378492D+00
11	0.125506D-02	-0.160745D-03	-0.725039D-03	0.328461D-02	0.330597D-02

Table 5b. Force Constant Matrix for Isopropanol [C_3H_8O] at the 6-31G* HF Level of Calculation. (CONTINUED 3)

12	-0.4176190-01	-0.4110260-02	-0.1057350-01	-0.8922090-02	0.1238090-01
13	-0.3472600-02	0.5510510-04	0.5843510-02	0.5750730-04	-0.6736530-03
14	-0.3438990-02	0.1180210-02	-0.8327030-03	0.6050310-03	0.1639540-02
15	0.1551090-01	-0.1371410-02	0.1100320-02	0.4830650-03	-0.5541380-03
16	-0.3405000-02	-0.9062250-02	-0.4636120-02	-0.5751010-02	0.6131270-02
17	0.4244240-01	0.1515610-01	0.6136030-03	0.9575420-03	0.2054570-03
18	-0.3389450-01	0.1141070-02	0.4319480-02	-0.7491570-03	0.1356480-02
19	0.1387360-01	0.1528270-02	0.5357900-03	-0.2271360-02	-0.8446850-02
20	-0.4192390-02	-0.5240110-03	-0.7830490-03	-0.9456270-02	-0.3981510-02
21	-0.3963390-02	-0.8761760-03	0.5577680-02	-0.9466680-02	-0.8962420-02
22	0.6199660-01	0.8839690-02	-0.1321880-01	0.9917470-02	-0.2646350-02
23	-0.6356130-03	-0.1901700-03	0.4327060-03	0.7742620-03	-0.8508210-04
24	-0.1436400-02	-0.3812000-03	-0.3491150-04	-0.2037660-04	0.2555460-03
25	-0.3421020-02	-0.1318980-01	0.8430290-02	-0.9449140-02	0.2146910-02
26	0.1285570-02	-0.5880080-03	-0.1718880-03	0.1233160-04	-0.2700330-03
27	-0.5696170-01	0.3877370-02	0.4831240-02	-0.4396740-03	0.2286870-03
28	-0.1824760-03	-0.8529060-04	0.1921150-03	-0.3906050-03	-0.1397160-01
29	0.5426260-03	0.2170770-03	-0.5336790-03	0.1520160-01	0.1145690-03
30	-0.1028330-02	-0.1987940-03	0.2027080-05	-0.1514380-01	0.1538140-01

	11	12	13	14	15
11	0.3754160+00				
12	-0.5320130-02	0.4004290+00			
13	0.1598730-02	-0.7276810-02	0.2518050+00		
14	0.5541670-03	0.3406420-01	0.3596090-01	0.2560110+00	
15	0.5385110-04	-0.2776830-02	0.3729150-01	0.3914240-01	0.2501690+00
16	-0.9721920-03	0.1133540+00	-0.1976890-01	-0.1264990-01	0.4684750-01
17	0.3071890-03	-0.1682920-01	0.5197280-03	0.4355400-02	-0.1187590-02
18	-0.3629990-02	0.6418690-01	0.3169230-01	-0.9063200-02	-0.7714280-02
19	-0.8594650-02	-0.2155150-01	0.4685090-03	-0.1262350-02	0.3529570-02
20	-0.9083250-02	0.4960810-01	-0.4872230-03	0.9775870-02	-0.1330640-02
21	-0.3702200-02	-0.1614580-01	0.2503010-02	-0.3656770-03	0.4687040-03
22	-0.1107820-01	-0.3886620-01	-0.2235270-02	0.6456230-01	-0.6259240-01
23	-0.7810310-03	-0.9290370-03	-0.6163430-01	-0.1244030-03	0.6343920-01
24	-0.1751980-04	-0.2966810-02	0.6444050-01	-0.6549430-01	-0.2323110-02
25	0.5973140-02	0.1083630+00	0.7821590-02	-0.3072780-02	0.1072070-02
26	0.2371940-03	-0.4536390-02	-0.8755280-03	-0.1011150-02	-0.9189230-03
27	0.5205890-02	-0.6617420-01	0.3423390-03	0.1582890-02	-0.1614860-02
28	0.1423690-01	0.7395390-02	-0.2459560-03	0.1578490-03	0.9641360-03
29	-0.1569210-01	0.1070350-02	0.1343740-02	0.2440710-03	-0.1052970-02
30	0.7413490-05	-0.3331590-02	-0.2684980-03	-0.3821420-03	-0.2767860-04

	16	17	18	19	20
16	0.4731020+00				
17	-0.1809860-01	0.2009420+00			
18	0.7397990-01	0.3935730-02	0.3037130+00		
19	-0.2340060-01	0.8623730-02	0.3584150-02	0.2541000+00	
20	0.1322400-01	-0.1385180-02	0.4705300-02	0.3724170-01	0.2532690+00
21	0.3511760-02	-0.1316830-02	-0.1621570-01	0.3706320-01	0.3519870-01
22	-0.1107360+00	0.2714610-01	0.6838070-01	0.3949790-01	-0.2257720-02
23	0.3406990-02	0.6562760-03	0.4219320-03	0.1089440-02	-0.2980590-03
24	-0.2780180-02	-0.2096610-02	-0.8236990-03	-0.9655690-03	-0.2080050-03
25	0.3263580-01	-0.3024690-01	-0.8188510-01	-0.3319480-01	0.9249290-02
26	-0.7804810-02	-0.3291800-03	0.2280720-02	0.5437300-03	-0.4934450-03
27	0.7911290-01	0.4003290-02	0.1404570-01	-0.6321740-02	-0.6636580-02
28	0.8970070-02	-0.1227400-03	-0.1123480-02	0.1387920-02	0.6424310-01
29	0.2251760-02	-0.2925160-03	-0.1631720-02	-0.6325850-01	0.4191440-02
30	0.1684130-02	0.3227520-03	-0.2446970-02	0.6331990-01	-0.6140210-01

	21	22	23	24	25
21	0.2546210+00				
22	-0.4365670-01	0.5364410+00			
23	-0.1394750-02	-0.1018800+00	0.2040540+00		
24	0.2237060-03	-0.1049300+00	-0.9663420-01	0.2026790+00	
25	0.1818730-01	-0.2213580+00	0.1361150-02	0.8262920-02	0.3876190+00
26	0.4633570-03	-0.1380440-03	-0.2332080-02	0.9299220-03	0.3636300-02
27	0.2569420-01	-0.1170110+00	0.1772760-02	0.4532180-03	-0.1610030+00
28	-0.6473180-01	0.4878010-02	0.7905520-04	-0.1644220-02	-0.4697500-02
29	0.6153790-01	0.2744450-02	-0.2188530-02	0.7453810-04	-0.8489700-03
30	-0.5640730-02	0.1329320-02	0.4329840-03	0.3728780-03	-0.7833200-03

	26	27	28	29	30
26	0.1088450-01				
27	-0.2416790-02	0.2813810+00			
28	-0.2429070-02	0.2043510-03	0.2036470+00		
29	0.6918800-04	-0.1477900-02	-0.9617470-01	0.2058790+00	
30	0.1332920-03	-0.2063690-02	-0.9682150-01	-0.1001580+00	0.2051080+00

Table 5c. Force Constant Matrix for Isopropanol [C_3H_8O] at the 6-31G* MP2 Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.612524D+00				
2	0.319145D-03	0.621683D+00			
3	0.142761D-02	-0.168485D-02	0.509288D+00		
4	-0.891727D-01	0.318398D-02	-0.638699D-03	0.581578D+00	
5	0.554355D-02	-0.863617D-01	-0.992797D-02	-0.570676D-01	0.573823D+00
6	-0.494327D-02	-0.196673D-01	-0.214311D+00	0.686389D-02	0.395376D-01
7	-0.149274D-03	0.178360D-02	-0.463439D-02	-0.203677D+00	0.660002D-02
8	0.180929D-03	0.185491D-02	-0.163538D-02	0.192800D-01	-0.852426D-01
9	-0.367674D-01	0.408934D-04	-0.174209D-01	-0.532469D-01	-0.227429D-02
10	-0.118542D+00	0.109502D+00	0.432067D-01	-0.323775D-03	0.104591D-03
11	0.109562D+00	-0.236880D+00	-0.741454D-01	0.326536D-03	-0.231225D-02
12	0.433404D-01	-0.720829D-01	-0.788217D-01	0.181328D-01	-0.328279D-01
13	-0.292151D+00	-0.411492D-02	-0.877339D-01	0.116859D-03	-0.118308D-02
14	-0.363844D-02	-0.531598D-01	-0.220707D-02	-0.149573D-02	-0.151373D-02
15	-0.873204D-01	-0.137336D-02	-0.832034D-01	-0.365991D-01	-0.297251D-03
16	-0.108768D+00	-0.102576D+00	0.448931D-01	-0.170347D-02	0.472276D-03
17	-0.101981D+00	-0.237682D+00	0.797791D-01	0.110243D-02	-0.181894D-05
18	0.439539D-01	0.784105D-01	-0.870805D-01	0.157602D-01	0.298611D-01
19	-0.302973D-02	-0.103179D-01	0.405341D-02	-0.117099D+00	-0.654121D-01
20	-0.117535D-01	-0.128555D-01	0.100283D-01	-0.273541D-01	-0.185991D+00
21	0.223454D-01	0.437413D-01	-0.170625D-01	-0.248759D-02	0.407336D-01
22	0.180037D-02	0.239157D-02	-0.101243D-05	-0.197855D-01	0.573731D-02
23	0.138782D-03	0.978911D-03	-0.581979D-03	-0.404921D-01	-0.576791D-02
24	0.295735D-02	0.102690D-03	0.165132D-02	0.176720D-01	0.444956D-02
25	0.182062D-02	0.530353D-03	-0.221746D-02	-0.122534D+00	0.102028D+00
26	0.199138D-02	0.207184D-02	-0.113293D-03	0.100095D+00	-0.203373D+00
27	0.189206D-01	-0.289664D-01	-0.145736D-01	0.443476D-01	-0.701959D-01
28	0.111938D-02	-0.108363D-03	0.914550D-03	-0.998114D-02	-0.273420D-01
29	0.208614D-03	-0.244910D-03	0.280881D-03	0.302077D-02	-0.179046D-03
30	0.129266D-03	-0.264386D-03	0.155889D-03	-0.459259D-02	-0.121540D-01
31	-0.679601D-02	-0.531000D-03	-0.124293D-02	0.164699D-02	0.388966D-03
32	0.150653D-05	0.346945D-03	-0.570263D-05	-0.184555D-03	-0.119242D-02
33	-0.369549D-02	0.270296D-03	0.891139D-04	0.260474D-02	0.536600D-03
34	0.134425D-02	-0.622436D-04	0.197249D-02	-0.190641D-01	0.301306D-01
35	-0.572886D-03	0.246801D-03	0.213769D-03	-0.415155D-03	-0.188756D-02
36	-0.347399D-03	0.147357D-02	0.128817D-02	-0.781708D-03	0.125585D-01

	6	7	8	9	10
6	0.539444D+00				
7	-0.487902D-01	0.535620D+00			
8	0.299297D-02	0.660447D-02	0.622422D+00		
9	-0.108291D+00	-0.354404D-01	-0.192355D-02	0.610580D+00	
10	0.148065D-03	0.773524D-03	-0.139103D-02	-0.569596D-03	0.122643D+00
11	0.833162D-03	-0.340081D-03	0.229150D-03	0.439662D-03	-0.120488D+00
12	-0.145784D-01	0.179519D-02	-0.459949D-03	0.195542D-02	-0.470566D-01
13	0.316393D-02	0.111944D-02	-0.446779D-03	-0.814183D-03	-0.137757D-01
14	0.284395D-03	0.145855D-03	0.470992D-03	-0.146450D-05	0.265374D-01
15	-0.120801D-01	0.203953D-02	0.240488D-03	-0.759743D-02	0.115481D-01
16	-0.897936D-03	-0.291070D-04	0.235332D-03	-0.354033D-03	0.863809D-02
17	-0.240872D-02	-0.166560D-03	-0.184911D-03	-0.327972D-03	-0.140732D-01
18	-0.479857D-02	0.419038D-03	0.234572D-03	0.153975D-02	-0.671959D-02
19	0.254530D-01	-0.267535D-01	-0.424255D-01	0.137606D-01	-0.268021D-03
20	0.600929D-01	-0.969757D-02	-0.718901D-02	0.352063D-02	-0.578328D-03
21	-0.943217D-01	-0.602873D-02	-0.965937D-02	0.643927D-02	-0.563992D-03
22	-0.112064D-01	-0.149840D-02	-0.595331D-02	0.254842D-02	-0.366371D-03
23	-0.126446D-01	-0.241470D-02	-0.616640D-02	0.264857D-02	0.520422D-03
24	0.259340D-02	0.868252D-03	0.131621D-02	-0.820399D-03	0.173212D-03
25	0.430921D-01	-0.177528D-01	0.269027D-01	0.109239D-01	0.991669D-03
26	-0.697813D-01	-0.177565D-03	0.229337D-02	-0.691059D-03	-0.295592D-03
27	-0.865509D-01	-0.912954D-02	0.106674D-01	0.492297D-02	-0.815915D-04
28	0.123850D-01	-0.120395D+00	-0.111185D+00	0.383500D-01	-0.322807D-04
29	0.114786D-03	-0.113184D+00	-0.239334D+00	0.648075D-01	-0.972735D-04
30	0.249299D-02	0.399021D-01	0.661395D-01	-0.755771D-01	-0.329759D-04

Table 5c. Force Constant Matrix for Isopropanol [C_3H_8O] at the 6-31G* MP2 Level of Calculation. (CONTINUED 1)

31	-0.3636940-01	-0.5171560-01	-0.9619320-04	0.1731200-01	-0.5388390-04
32	0.1168610-02	0.5881160-03	-0.5328930-01	0.6869350-02	0.4149290-05
33	-0.1340410-01	0.1421780-01	0.6381810-02	-0.3331020+00	0.7057560-04
34	0.1110110-01	-0.1155430+00	0.1082940+00	0.4429820-01	0.3160090-03
35	-0.5219870-03	0.1102580+00	-0.2358650+00	-0.7310830-01	0.2555320-03
36	0.3805350-02	0.4478050-01	-0.7429480-01	-0.8263020-01	-0.1221990-03
	11	12	13	14	15
11	0.2524160+00				
12	0.8182480-01	0.8643750-01			
13	-0.2557580-02	-0.5601130-02	0.3143600+00		
14	0.2143250-02	0.1083180-01	0.5134010-02	0.5049770-01	
15	0.1146170-02	0.3839590-02	0.9737390-01	0.1728110-02	0.9045740-01
16	0.1457100-01	-0.7651390-02	-0.1309300-01	-0.2681810-01	0.1274900-01
17	-0.1923800-01	0.1055180-01	0.1689970-02	0.6514040-03	-0.6308570-03
18	-0.9732350-02	0.4104030-02	-0.5422430-02	-0.1109800-01	0.4471820-02
19	0.2490810-04	-0.2015190-02	0.2337940-02	0.9614130-03	0.2625720-03
20	0.2100270-02	0.7042530-03	0.1421580-02	-0.5456640-04	-0.1975100-02
21	0.2734610-03	0.4533500-02	0.3285160-03	-0.1725520-03	0.3673250-02
22	-0.1355580-03	0.2569200-03	-0.4580230-04	-0.2420260-03	0.1090250-02
23	-0.9320140-04	-0.8659590-04	0.3857500-03	0.1830460-03	0.1066120-02
24	-0.1352220-03	-0.2584810-03	-0.1037510-02	0.6543300-03	-0.8293570-03
25	-0.3856370-03	-0.5353320-04	0.6650210-03	-0.4750310-03	0.6568130-03
26	0.1273670-02	0.4349790-03	-0.1957170-03	-0.2102940-03	0.1093210-03
27	-0.1106760-03	-0.7437410-02	-0.6519700-03	0.1108420-03	0.1830160-02
28	0.6922000-04	-0.1001670-03	0.1421670-03	0.4175150-03	0.2674590-03
29	-0.4015920-04	0.4889370-04	0.1337130-03	0.2021450-03	-0.1967620-03
30	-0.9896560-04	-0.9661220-05	0.1988020-03	0.7886850-04	0.1907960-03
31	-0.2000020-03	0.1725430-04	-0.6585240-05	-0.9297990-04	-0.2223780-02
32	0.2254370-03	0.4499110-03	-0.3305390-04	0.5670160-03	0.4860370-04
33	0.1523000-03	0.3862190-03	-0.7471970-04	-0.2901700-04	-0.8031630-03
34	-0.4456970-03	-0.1064360-02	0.3310130-03	-0.4337180-03	0.1561760-03
35	0.1751410-03	0.6105620-03	-0.2342020-03	0.2234630-03	0.1343600-03
36	-0.4473840-03	-0.1505900-03	0.2699740-03	-0.1802640-03	0.5128200-04
	16	17	18	19	20
16	0.1128680+00				
17	0.1131300+00	0.2539710+00			
18	-0.4828380-01	-0.8855200-01	0.9109210-01		
19	0.1555560-02	-0.5441070-03	0.2009440-02	0.5662550+00	
20	0.2081960-03	0.1908870-02	0.3241590-02	0.9831990-01	0.2706720+00
21	0.3652590-03	0.1201880-02	-0.1011790-01	0.1434260+00	-0.1010840+00
22	0.5837290-03	0.3111250-03	-0.1022380-02	-0.4297000+00	-0.2823020-01
23	0.3405180-03	-0.1641990-03	-0.4169630-03	0.1852180-01	-0.3273550-01
24	-0.6646320-03	-0.2941500-03	-0.2074810-03	-0.1815810+00	0.8241490-02
25	-0.1441090-03	0.1539150-03	-0.2705090-04	0.9396630-02	-0.2296340-01
26	0.2103930-03	0.1326960-03	-0.1253050-02	0.1691090-02	-0.3847380-01
27	0.1680700-03	0.5860480-03	0.1233800-02	-0.4812360-02	0.1767290-01
28	0.9177440-04	0.2719860-03	-0.8424640-03	-0.8317570-02	-0.3806610-03
29	0.4233580-04	0.4772940-03	-0.2831350-03	-0.5008590-03	0.1150470-02
30	-0.4549210-03	0.5911100-04	-0.4576160-03	-0.3269890-02	-0.3989370-03
31	-0.2412600-04	0.1918970-03	0.2530020-03	0.2406840-02	0.1278830-02
32	0.7270110-04	0.1624290-03	-0.3964840-03	-0.1404840-03	0.2063020-04
33	0.1300150-03	-0.4223070-04	0.2968170-03	0.1035670-02	-0.2940670-04
34	0.2521790-04	-0.8769060-04	-0.7789540-04	0.3215580-02	-0.2709840-03
35	0.1116120-03	-0.3340850-04	-0.1575630-04	-0.1775950-03	0.1448110-02
36	0.1419540-05	0.7867560-04	-0.7622390-04	0.1678220-02	-0.1441150-04
	21	22	23	24	25
21	0.1805310+00				
22	-0.1521850+00	0.4472930+00			
23	0.2641550-01	0.2453460-01	0.4287090-01		
24	-0.8119750-01	0.1615900+00	-0.1530220-01	0.7836300-01	
25	-0.2942790-02	0.1656460-02	0.3121960-04	-0.4516800-03	0.1294290+00
26	-0.2463320-03	0.1546450-02	0.3379650-03	0.5383950-03	-0.1050160+00
27	0.6522790-02	-0.6547020-03	-0.9532990-03	-0.3162740-03	-0.4655140-01
28	-0.3355360-02	-0.9689720-03	-0.1924670-02	0.4223860-03	0.1013470-02
29	-0.3247590-03	-0.2801710-05	0.5239600-03	0.3036750-03	-0.4372890-03
30	-0.3717480-03	-0.6716610-03	-0.5029400-03	0.8428230-03	0.6141590-03

Table 5c. Force Constant Matrix for Isopropanol [C_3H_8O] at the 6-31G* MP2 Level of Calculation. (CONTINUED 2)

31	0.126082D-02	0.332348D-03	0.364127D-03	0.100920D-03	0.160304D-02
32	-0.766459D-03	0.122397D-03	-0.113867D-03	0.137702D-03	-0.328346D-03
33	0.154596D-02	0.186567D-03	0.860444D-04	0.312582D-03	-0.334737D-04
34	-0.163801D-03	0.699035D-03	-0.575346D-05	-0.486121D-04	-0.614554D-02
35	-0.112000D-03	-0.795082D-04	0.147093D-03	-0.131735D-04	-0.407407D-04
36	-0.174559D-03	0.685418D-04	0.271980D-03	-0.133460D-03	-0.300928D-02

	26	27	28	29	30
26	0.234646D+00				
27	0.706022D-01	0.937900D-01			
28	0.846812D-03	0.605735D-03	0.128392D+00		
29	0.306525D-03	-0.328745D-03	0.124591D+00	0.255926D+00	
30	0.177707D-03	0.121332D-03	-0.420711D-01	-0.721630D-01	0.762865D-01
31	-0.269325D-04	0.724468D-03	-0.927038D-03	0.132281D-02	0.173824D-01
32	-0.233714D-03	0.469185D-03	0.123328D-03	0.656900D-03	0.289656D-01
33	0.182445D-03	0.760017D-03	-0.269820D-03	-0.128140D-02	-0.650154D-02
34	-0.669589D-03	-0.288473D-02	0.986354D-02	-0.150973D-01	-0.713382D-02
35	0.122896D-02	0.446324D-03	0.146209D-01	-0.194444D-01	-0.983846D-02
36	0.399183D-04	-0.302989D-03	-0.630615D-02	0.902284D-02	0.282749D-02

	31	32	33	34	35
31	0.543407D-01				
32	-0.686022D-03	0.507425D-01			
33	-0.139650D-01	-0.803247D-02	0.358964D+00		
34	-0.805496D-03	0.460487D-03	-0.207226D-03	0.125763D+00	
35	-0.191335D-02	0.210808D-02	0.180530D-02	-0.121812D+00	0.251652D+00
36	0.167509D-01	-0.289079D-01	-0.854414D-02	-0.459472D-01	0.803990D-01

	36
36	0.840399D-01

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.303895D+00				
2	0.100191D-01	0.319045D+00			
3	0.400252D-02	0.519428D-03	0.357257D+00		
4	0.426694D-02	-0.183615D-03	0.117023D-02	0.350860D+00	
5	0.284859D-02	-0.100896D-03	0.837109D-03	0.123065D-02	0.355244D+00
6	0.185367D-01	0.169195D-01	0.756583D-03	0.215415D-02	0.824462D-03
7	0.430703D-03	0.584912D-04	0.340376D-04	-0.117422D-03	-0.662646D-03
8	0.608009D-02	0.535625D-02	-0.628313D-03	0.516816D-03	0.531847D-03
9	-0.308056D-04	0.241640D-02	-0.632362D-04	-0.935974D-04	0.700246D-03
10	-0.932047D-04	0.331440D-02	-0.214966D-03	0.325380D-03	-0.934637D-04
11	0.630061D-03	0.426868D-02	0.497522D-03	-0.226115D-03	-0.684608D-04
12	0.434301D-01	0.316437D-03	-0.323241D-02	0.788348D-02	-0.256230D-02
13	0.311714D-01	-0.351850D-02	-0.373213D-02	-0.887819D-02	-0.868519D-02
14	0.311153D-01	0.655540D-02	-0.833140D-02	-0.504548D-02	-0.897738D-02
15	0.256271D-01	-0.512301D-03	-0.794882D-02	-0.910888D-02	-0.341024D-02
16	0.346257D-01	-0.246981D-01	-0.571649D-02	-0.167985D-02	0.109582D-01
17	-0.246131D-03	0.563094D-02	-0.263134D-03	0.239876D-02	-0.957837D-03
18	0.373486D-01	-0.210051D-01	0.604952D-02	-0.480334D-03	-0.147165D-03
19	-0.362874D-03	0.273985D-01	0.288597D-04	-0.624006D-03	0.617946D-03
20	0.659221D-02	0.315089D-01	0.244197D-03	0.168685D-02	0.111095D-03
21	-0.339225D-02	0.318247D-01	0.169256D-02	-0.780931D-03	0.627121D-04
22	0.488298D-03	0.612067D-02	-0.298639D-02	-0.140026D-01	0.151150D-01
23	0.138794D-02	-0.806892D-04	0.143989D-01	0.904528D-04	-0.144586D-01
24	-0.181166D-02	-0.434619D-03	-0.135199D-01	0.150143D-01	0.775811D-03
25	0.384735D-02	-0.342277D-01	0.243175D-02	-0.300372D-02	-0.100915D-03
26	0.298103D-03	0.322542D-03	-0.795250D-03	-0.127350D-02	0.992740D-03
27	-0.359801D-02	0.277967D-01	-0.185339D-04	0.127670D-02	-0.785349D-03
28	0.484028D-03	0.429135D-03	0.101440D-03	-0.300850D-03	0.125827D-03
29	0.251171D-03	0.634517D-04	0.655150D-03	-0.747495D-05	-0.592608D-03
30	0.149690D-03	-0.753614D-03	-0.215448D-03	0.350968D-03	-0.134630D-03

	6	7	8	9	10
6	0.349721D+00				
7	-0.319153D-02	0.508526D+00			
8	0.150943D-01	-0.410441D-03	0.329707D+00		
9	0.773709D-03	0.205974D-03	0.516978D-03	0.356965D+00	
10	0.162933D-03	-0.269886D-03	0.431980D-03	0.102561D-02	0.359799D+00
11	0.582441D-03	-0.367910D-03	-0.638430D-03	0.935911D-03	0.111715D-02

Table 5c. Force Constant Matrix for Isopropanol [C_3H_8O] at the 6-31G* MP2 Level of Calculation. (CONTINUED 3)

12	-0.3893510-01	-0.5484470-02	-0.1063830-01	-0.7725420-02	0.1164600-01
13	-0.4461390-02	0.2918400-03	0.4981490-02	0.6287100-04	-0.6605440-03
14	-0.4295170-02	0.1730770-02	-0.1226560-02	0.2532420-03	0.1327290-02
15	0.1360560-01	-0.1766950-02	0.8938920-03	0.6012870-03	-0.5832940-03
16	-0.3310490-02	-0.1052000-01	-0.3733750-02	-0.4981070-02	0.5257920-02
17	0.4931170-01	0.1741360-01	0.5074710-03	0.9121620-03	0.1011960-03
18	-0.3115450-01	0.1935470-02	0.5334060-02	-0.3723400-03	0.1269790-02
19	0.1171030-01	0.1732270-02	0.2907220-03	-0.2310650-02	-0.7989070-02
20	-0.4273700-02	-0.7561330-03	-0.1131130-02	-0.8963020-02	-0.3730340-02
21	-0.4513660-02	-0.1032500-02	0.4703660-02	-0.8734550-02	-0.8260570-02
22	0.5917670-01	0.1116970-01	-0.1335280-01	0.9431480-02	-0.2601730-02
23	-0.3813490-03	-0.4271550-04	0.2156450-03	0.6761180-03	-0.7490540-04
24	-0.1584180-02	-0.3570980-03	0.2898310-03	-0.1215900-03	0.2678750-03
25	-0.5674190-02	-0.1579050-01	0.6742020-02	-0.8720670-02	0.2370730-02
26	0.1245140-02	-0.6234940-03	-0.5948420-03	-0.1218350-03	-0.3975230-03
27	-0.5226840-01	0.3995300-02	0.6691660-02	-0.5958580-03	-0.4353670-04
28	-0.1490690-03	-0.1002990-03	-0.1015130-03	-0.2984560-03	-0.1351640-01
29	0.2216000-03	0.3199060-03	-0.2747290-03	0.1458490-01	-0.2746650-03
30	-0.5601020-03	-0.2959180-03	-0.4484030-04	-0.1447460-01	0.1473810-01

	11	12	13	14	15
11	0.3571860+00				
12	-0.5002790-02	0.3694360+00			
13	0.1765500-02	-0.6558120-02	0.2285330+00		
14	0.2855620-03	0.3072490-01	0.3113270-01	0.2315730+00	
15	0.5819550-04	-0.2547410-02	0.3225640-01	0.3562650-01	0.2247640+00
16	-0.3006330-03	0.9995820-01	-0.1838280-01	-0.1058260-01	0.4196370-01
17	0.2340510-03	-0.1592490-01	0.5737240-03	0.4212700-02	-0.9841450-03
18	-0.3261310-02	0.5822130-01	0.2821380-01	-0.7966400-02	-0.6864200-02
19	-0.7869680-02	-0.1846870-01	0.4323750-03	-0.1213530-02	0.3262970-02
20	-0.8368010-02	0.4500490-01	-0.3465680-03	0.8968950-02	-0.1282580-02
21	-0.3000470-02	-0.1502480-01	0.2197080-02	-0.2550610-03	0.4387440-03
22	-0.1027160-01	-0.3392450-01	-0.2940580-02	0.5891990-01	-0.5664250-01
23	-0.6625520-03	-0.5768310-03	-0.5690480-01	0.6196000-03	0.5870030-01
24	-0.9366480-04	-0.2825300-02	0.5975930-01	-0.6090050-01	-0.2792500-02
25	0.5707660-02	0.9878180-01	0.8086800-02	-0.2748770-02	0.1138100-02
26	0.3642910-03	-0.4421850-02	-0.6949620-03	-0.7855670-03	-0.1001310-02
27	0.4801800-02	-0.6105820-01	0.7844740-03	0.1683950-02	-0.2292970-02
28	0.1377130-01	0.7419910-02	-0.2831450-03	0.3684620-03	0.8667630-03
29	-0.1509280-01	0.7806670-03	0.1470800-02	0.2273060-03	-0.1205720-02
30	0.2217860-03	-0.3994140-02	-0.1981560-03	-0.6205180-03	-0.8148780-05

	16	17	18	19	20
16	0.4298490+00				
17	-0.1809160-01	0.1895940+00			
18	0.6422370-01	0.2772430-02	0.2752770+00		
19	-0.2030200-01	0.8347070-02	0.2740930-02	0.2283870+00	
20	0.1247230-01	-0.1199090-02	0.4266990-02	0.3335760-01	0.2286110+00
21	0.1671210-02	-0.1157800-02	-0.1410270-01	0.3197280-01	0.3058880-01
22	-0.1022100+00	0.2617410-01	0.6266650-01	0.3487730-01	-0.1466950-02
23	0.4203640-02	0.7713280-03	0.3698420-03	0.1228270-02	-0.3524700-03
24	-0.3632640-02	-0.2118670-02	-0.7869100-03	-0.7993040-03	-0.4315550-03
25	0.3128000-01	-0.2748660-01	-0.7201410-01	-0.2906940-01	0.7537810-02
26	-0.6694010-02	-0.1611870-04	0.2486330-02	0.3914930-03	-0.6168750-03
27	0.7124890-01	0.2169140-02	0.9832340-02	-0.5798820-02	-0.5502070-02
28	0.8392330-02	-0.1747080-03	-0.1046920-02	0.1466630-02	0.5972970-01
29	0.2818250-02	-0.5281040-03	-0.1854000-02	-0.5868970-01	0.4327540-02
30	0.1417740-02	0.5006240-03	-0.2009290-02	0.5812080-01	-0.5618670-01

	21	22	23	24	25
21	0.2310380+00				
22	-0.3970670-01	0.4997690+00			
23	-0.1536480-02	-0.9500180-01	0.1882330+00		
24	0.2612690-03	-0.9712670-01	-0.8772410-01	0.1860670+00	
25	0.1688120-01	-0.2104120+00	0.2099200-02	0.8155740-02	0.3569540+00
26	0.6577130-03	-0.1731080-02	-0.2387870-02	0.9192960-03	0.5453710-02
27	0.2301890-01	-0.1064810+00	0.1992340-02	0.4155180-03	-0.1403080+00
28	-0.6004640-01	0.5303150-02	0.7046990-04	-0.1570030-02	-0.5019520-02
29	0.5674920-01	0.2621280-02	-0.2125020-02	0.3781060-04	-0.5759190-03
30	-0.5926210-02	0.1997380-02	0.4505810-03	0.4074420-03	-0.1746540-02

	26	27	28	29	30
26	0.1189950-01				
27	-0.2385000-02	0.2497200+00			
28	-0.2946060-02	0.1552160-03	0.1869130+00		
29	0.5601300-04	-0.1578760-02	-0.8745680-01	0.1897190+00	
30	0.1691910-03	-0.1908390-02	-0.8914630-01	-0.9245460-01	0.1898400+00

Table 5d. Force Constant Scaling Constants, Q(I), and C matrix for Isopropanol [C_3H_8O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation.

Q Values

I	Q(I)
1	0.962142E+00
2	0.969243E+00
3	0.951906E+00
4	0.953038E+00
5	0.949910E+00
6	0.866173E+00
7	0.839952E+00
8	0.927179E+00
9	0.953456E+00
10	0.950612E+00
11	0.951441E+00
12	0.922600E+00
13	0.907579E+00
14	0.904544E+00
15	0.898446E+00
16	0.908575E+00
17	0.943528E+00
18	0.906370E+00
19	0.898807E+00
20	0.902638E+00
21	0.907381E+00
22	0.931638E+00
23	0.922470E+00
24	0.918036E+00
25	0.920889E+00
26	0.109325E+01
27	0.887480E+00
28	0.917830E+00
29	0.921506E+00
30	0.925561E+00

C Matrix (30,30)

		COLUMN 1	COLUMN 2	COLUMN 3
ROW	1	0.1000000000000D+01		
ROW	2	0.9205613488220+00	0.1000000000000+01	
ROW	3	0.1076957624630+01	0.1000000000000+01	0.1000000000000+01
ROW	4	0.1015537120410+01	0.1000000000000+01	0.3487665547570+00
ROW	5	0.1144668480500+01	0.1000000000000+01	0.2811639741050+00
ROW	6	0.9743056235030+00	0.1029939260850+01	0.5270864515930+00
ROW	7	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	8	0.8731009598100+00	0.8500556344130+00	0.1000000000000+01
ROW	9	0.1000000000000+01	0.9458179486340+00	0.1000000000000+01
ROW	10	0.1000000000000+01	0.1009663461280+01	0.1000000000000+01
ROW	11	0.1000000000000+01	0.1040544552370+01	0.1000000000000+01
ROW	12	0.1060958403080+01	0.1000000000000+01	0.1064669214270+01
ROW	13	0.1097760475610+01	0.1404727855460+01	0.8918503728670+00
ROW	14	0.1119453648010+01	0.1083092566270+01	0.9795038943740+00
ROW	15	0.1104699411580+01	0.1000000000000+01	0.9889048578540+00
ROW	16	0.1024892794850+01	0.1084314818100+01	0.1141503159620+01
ROW	17	0.1000000000000+01	0.1028611477460+01	0.1000000000000+01
ROW	18	0.1091577999680+01	0.1098995805620+01	0.9844617262610+00
ROW	19	0.1000000000000+01	0.1109398798070+01	0.1000000000000+01
ROW	20	0.1039009902470+01	0.1089989881890+01	0.1000000000000+01
ROW	21	0.1428792655710+01	0.1082150270310+01	0.1182824298580+01
ROW	22	0.3486033644930+00	0.1112200376770+01	0.1000598301550+01
ROW	23	0.1335081185420+01	0.1000000000000+01	0.1031610197970+01
ROW	24	0.1175173656200+01	0.1000000000000+01	0.1026143233570+01
ROW	25	0.1445410803420+01	0.1080088203950+01	0.9108588336120+00

Table 5d. Force Constant Scaling Constants, Q(I), and C matrix for Isopropanol [C_3H_8O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED 1)

ROW	26	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	27	0.1163810183440+01	0.1098057912010+01	0.1000000000000+01
ROW	28	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	29	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	30	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 4	COLUMN 5	COLUMN 6
ROW	4	0.1000000000000+01		
ROW	5	0.3567457303830+00	0.1000000000000+01	
ROW	6	0.8008309104990+00	0.8013147202380+00	0.1000000000000+01
ROW	7	0.1000000000000+01	0.1000000000000+01	0.2207828320680+01
ROW	8	0.5148932458810+00	0.5211454652520+00	0.9053478210110+00
ROW	9	0.1000000000000+01	0.6792205393200+00	0.7732472553700+00
ROW	10	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	11	0.1000000000000+01	0.1000000000000+01	0.5112062470730+00
ROW	12	0.1007152798680+01	0.1000927030410+01	0.1042922677930+01
ROW	13	0.9857777254160+00	0.9984239894560+00	0.1449006936070+01
ROW	14	0.1108209210400+01	0.1018280593180+01	0.1411017534560+01
ROW	15	0.1022819989540+01	0.1178765010540+01	0.9943344706030+00
ROW	16	0.1014526857520+01	0.1041746688690+01	0.1095952953300+01
ROW	17	0.1100560673510+01	0.9681354697230+00	0.1285200298600+01
ROW	18	0.1000000000000+01	0.1000000000000+01	0.1037377869110+01
ROW	19	0.1000000000000+01	0.1000000000000+01	0.9566319631840+00
ROW	20	0.9275905872970+00	0.1000000000000+01	0.1152876238850+01
ROW	21	0.1000000000000+01	0.1000000000000+01	0.1284591815500+01
ROW	22	0.1038195081480+01	0.1008851304770+01	0.1062569382040+01
ROW	23	0.1000000000000+01	0.1030629593280+01	0.1000000000000+01
ROW	24	0.1029078567830+01	0.1000000000000+01	0.1236792282130+01
ROW	25	0.9022736615290+00	0.1000000000000+01	0.1857128445220+01
ROW	26	0.9982606542150+00	0.9333945427120+00	0.9953149979180+00
ROW	27	0.9582975854360+00	0.8525722916390+00	0.1046585284200+01
ROW	28	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	29	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	30	0.1000000000000+01	0.1000000000000+01	0.6083201014240+00

		COLUMN 7	COLUMN 8	COLUMN 9
ROW	7	0.1000000000000+01		
ROW	8	0.1000000000000+01	0.1000000000000+01	
ROW	9	0.1000000000000+01	0.5350693176600+00	0.1000000000000+01
ROW	10	0.1000000000000+01	0.1000000000000+01	0.3236710802200+00
ROW	11	0.1000000000000+01	0.1000000000000+01	0.2991646044740+00
ROW	12	0.1515763672640+01	0.1087834449890+01	0.9232051747840+00
ROW	13	0.1000000000000+01	0.9293108075710+00	0.1000000000000+01
ROW	14	0.1682436963100+01	0.1000000000000+01	0.1000000000000+01
ROW	15	0.1483139698410+01	0.8900996834260+00	0.1000000000000+01
ROW	16	0.1328836795460+01	0.8774631463420+00	0.9305668751510+00
ROW	17	0.1290615886170+01	0.1000000000000+01	0.1000000000000+01
ROW	18	0.1943990463070+01	0.1347075060790+01	0.1000000000000+01
ROW	19	0.1304536445870+01	0.1000000000000+01	0.1098920389370+01
ROW	20	0.1000000000000+01	0.1000000000000+01	0.1021710387800+01
ROW	21	0.1000000000000+01	0.9194012548610+00	0.9919684810630+00
ROW	22	0.1428407148790+01	0.1086868269730+01	0.1009032202640+01
ROW	23	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	24	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	25	0.1361211897020+01	0.8654903388210+00	0.9849262536900+00
ROW	26	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	27	0.1193454058150+01	0.1526911734060+01	0.1000000000000+01
ROW	28	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	29	0.1000000000000+01	0.1000000000000+01	0.1023559740490+01
ROW	30	0.1000000000000+01	0.1000000000000+01	0.1017467546600+01

		COLUMN 10	COLUMN 11	COLUMN 12
ROW	10	0.1000000000000+01		
ROW	11	0.3553207053580+00	0.1000000000000+01	
ROW	12	0.1004414299860+01	0.1003673541340+01	0.1000000000000+01
ROW	13	0.1000000000000+01	0.1188388832020+01	0.9848942810860+00

Table 5d. Force Constant Scaling Constants, Q(I), and C matrix for Isopropanol [C_3H_8O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED 2)

ROW	14	0.873028896964D+00	0.100000000000D+01	0.987347054663D+00
ROW	15	0.100000000000D+01	0.100000000000D+01	0.100762259824D+01
ROW	16	0.922744702138D+00	0.100000000000D+01	0.963151781189D+00
ROW	17	0.100000000000D+01	0.100000000000D+01	0.101421315598D+01
ROW	18	0.100847326223D+01	0.967480397867D+00	0.991918361927D+00
ROW	19	0.102321376861D+01	0.990158123347D+00	0.941066343140D+00
ROW	20	0.101144357749D+01	0.994107580995D+00	0.994131557353D+00
ROW	21	0.992403345396D+00	0.872257454903D+00	0.101706389100D+01
ROW	22	0.104469551771D+01	0.984822209016D+00	0.941478677903D+00
ROW	23	0.100000000000D+01	0.100000000000D+01	0.100000000000D+01
ROW	24	0.100000000000D+01	0.100000000000D+01	0.103475407241D+01
ROW	25	0.118022174416D+01	0.102084816444D+01	0.988971280198D+00
ROW	26	0.100000000000D+01	0.100000000000D+01	0.970570615935D+00
ROW	27	0.100000000000D+01	0.100378029328D+01	0.101969279255D+01
ROW	28	0.103569894126D+01	0.103511227538D+01	0.109030908646D+01
ROW	29	0.100000000000D+01	0.102718173972D+01	0.791015361586D+00
ROW	30	0.102150656801D+01	0.100000000000D+01	0.129736692630D+01

		COLUMN 13	COLUMN 14	COLUMN 15
ROW	13	0.100000000000D+01		
ROW	14	0.955496252379D+00	0.100000000000D+01	
ROW	15	0.957895308766D+00	0.100963653442D+01	0.100000000000D+01
ROW	16	0.102401792996D+01	0.922804145793D+00	0.991427894015D+00
ROW	17	0.100000000000D+01	0.104698628787D+01	0.900053963026D+00
ROW	18	0.981551868743D+00	0.970761342371D+00	0.986042987065D+00
ROW	19	0.100000000000D+01	0.106616424578D+01	0.102875234536D+01
ROW	20	0.100000000000D+01	0.101534709715D+01	0.107033496313D+01
ROW	21	0.967268564157D+00	0.100000000000D+01	0.100000000000D+01
ROW	22	0.143066531989D+01	0.994132812939D+00	0.989125180742D+00
ROW	23	0.100903962077D+01	0.100000000000D+01	0.101638934688D+01
ROW	24	0.101595521836D+01	0.102040355184D+01	0.132357252716D+01
ROW	25	0.113093008033D+01	0.980143083043D+00	0.116709737337D+01
ROW	26	0.100000000000D+01	0.781255158543D+00	0.100000000000D+01
ROW	27	0.100000000000D+01	0.118736786551D+01	0.159014624946D+01
ROW	28	0.100000000000D+01	0.100000000000D+01	0.100000000000D+01
ROW	29	0.119686595624D+01	0.100000000000D+01	0.125844448900D+01
ROW	30	0.100000000000D+01	0.100000000000D+01	0.100000000000D+01

		COLUMN 16	COLUMN 17	COLUMN 18
ROW	16	0.100000000000D+01		
ROW	17	0.107963080151D+01	0.100000000000D+01	
ROW	18	0.956639794736D+00	0.761736818836D+00	0.100000000000D+01
ROW	19	0.960059883692D+00	0.105106154007D+01	0.847277932994D+00
ROW	20	0.104146732448D+01	0.938017[illegible]D+00	0.100259278815D+01
ROW	21	0.524121144435D+00	0.950238[illegible]D+00	0.959002036707D+00
ROW	22	0.100322829732D+01	0.102840[illegible]D+01	0.997299166958D+00
ROW	23	0.134771572452D+01	0.100000[illegible]D+01	0.100000000000D+01
ROW	24	0.143066860391D+01	0.108576793[illegible]D+01	0.100000000000D+01
ROW	25	0.104782295140D+01	0.974899019910D+00	0.962623503990D+00
ROW	26	0.860566721421D+00	0.100000000000D+01	0.109515494268D+01
ROW	27	0.100293044847D+01	0.592125165085D+00	0.780515814437D+00
ROW	28	0.102453151552D+01	0.100000000000D+01	0.102168286944D+01
ROW	29	0.136781773524D+01	0.100000000000D+01	0.124326236588D+01
ROW	30	0.917988453202D+00	0.100000000000D+01	0.896516236244D+00

		COLUMN 19	COLUMN 20	COLUMN 21
ROW	19	0.100000000000D+01		
ROW	20	0.994431568948D+00	0.100000000000D+01	
ROW	21	0.955232533945D+00	0.960249803509D+00	0.100000000000D+01
ROW	22	0.964964960437D+00	0.708542858548D+00	0.989224544779D+00
ROW	23	0.123817505745D+01	0.100000000000D+01	0.120409034858D+01
ROW	24	0.100000000000D+01	0.100000000000D+01	0.100000000000D+01
ROW	25	0.962562301769D+00	0.893874341207D+00	0.101539891275D+01
ROW	26	0.100000000000D+01	0.100000000000D+01	0.100000000000D+01
ROW	27	0.102704760949D+01	0.926288140609D+00	0.998333307980D+00
ROW	28	0.116343234991D+01	0.102146991242D+01	0.101646643944D+01

Table 5d. Force Constant Scaling Constants, Q(I), and C matrix for Isopropanol [C_3H_8O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED 3)

ROW	29	0.101943704275D+01	0.113206574131D+01	0.100849485994D+01
ROW	30	0.100636595858D+01	0.100113205356D+01	0.114642151801D+01

		COLUMN 22	COLUMN 23	COLUMN 24
ROW	22	0.100000000000D+01		
ROW	23	0.100587689106D+01	0.100000000000D+01	
ROW	24	0.100088579185D+01	0.986465617501D+00	0.100000000000D+01
ROW	25	0.102624053900D+01	0.167327088110D+01	0.107348522767D+01
ROW	26	0.100000000000D+01	0.101960722575D+01	0.100000000000D+01
ROW	27	0.100078717601D+01	0.124210142184D+01	0.100000000000D+01
ROW	28	0.117567231140D+01	0.100000000000D+01	0.104025379881D+01
ROW	29	0.103082644274D+01	0.105313733791D+01	0.100000000000D+01
ROW	30	0.161809317976D+01	0.100000000000D+01	0.100000000000D+01

		COLUMN 25	COLUMN 26	COLUMN 27
ROW	25	0.100000000000D+01		
ROW	26	0.149475368191D+01	0.100000000000D+01	
ROW	27	0.963971130230D+00	0.100186663399D+01	0.100000000000D+01
ROW	28	0.116227961337D+01	0.121076588983D+01	0.100000000000D+01
ROW	29	0.100000000000D+01	0.100000000000D+01	0.118125637726D+01
ROW	30	0.100000000000D+01	0.100000000000D+01	0.102032883997D+01

		COLUMN 28	COLUMN 29	COLUMN 30
ROW	28	0.100000000000D+01		
ROW	29	0.988786526494D+00	0.100000000000D+01	
ROW	30	0.998959377175D+00	0.999520869962D+00	0.100000000000D+01

Table 6a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Dimethyl ether [C_2H_6O] Based on Several Levels of Calculation.

H5 H4

H6 C1 O2 C3 H8

H7 H9

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
geometry					
$r(C_1\text{-}O_2)$/A	1.4328	1.4664	1.3912	1.4156	-
$r(O_2\text{-}C_3)$/A	1.4328	1.4664	1.3912	1.41560	-
$r(C_3\text{-}H_4)$/A	1.0862	1.0994	1.0889	1.0993	-
$r(C_1\text{-}H_5)$/A	1.0838	1.0966	1.0813	1.0906	-
$r(C_1\text{-}H_6)$/A	1.0838	1.0966	1.0889	1.0993	-
$r(C_1\text{-}H_7)$/A	1.0838	1.0966	1.0889	1.0993	-
$r(C_3\text{-}H_8)$/A	1.0827	1.0952	1.0889	1.0993	-
$r(C_3\text{-}H_9)$/A	1.0827	1.0952	1.0813	1.0906	-
$\phi(C_3\text{-}O_2\text{-}C_1)$/°	113.9529	110.3900	113.8089	111.0515	-
$\phi(H_4\text{-}C_3\text{-}O_2)$/°	111.4661	111.7822	111.4933	111.4693	-
$\phi(H_5\text{-}C_1\text{-}O_2)$/°	106.8360	105.9936	107.6459	106.8894	-
$\phi(H_6\text{-}C_1\text{-}O_2)$/°	111.4796	111.7978	111.4936	111.4695	-
$\phi(H_7\text{-}C_1\text{-}O_2)$/°	111.4741	111.7889	111.4935	111.4695	-
$\phi(H_8\text{-}C_3\text{-}O_2)$/°	111.4859	111.8040	111.4937	111.4696	-
$\phi(H_9\text{-}C_3\text{-}O_2)$/°	106.8424	106.0009	107.6461	106.8899	-
$\tau(H_4\text{-}C_3\text{-}O_2\text{-}C_1)$/°	60.7441	60.8520	60.6567	60.6961	-
$\tau(H_5\text{-}C_1\text{-}O_2\text{-}C_3)$/°	-180.0013	-179.9989	-180.0038	-180.0030	-
$\tau(H_6\text{-}C_1\text{-}O_2\text{-}C_3)$/°	60.7694	60.8817	60.6523	60.6938	-
$\tau(H_7\text{-}C_1\text{-}O_2\text{-}C_3)$/°	-60.7722	-60.8801	-60.6598	-60.6995	-
$\tau(H_8\text{-}C_3\text{-}O_2\text{-}C_1)$/°	-60.7705	-60.8756	-60.6552	-60.6968	-
$\tau(H_9\text{-}C_3\text{-}O_2\text{-}C_1)$/°	-180.0531	-180.0607	-179.9993	-180.0008	-
E/a.u.	-153.213171	-153.520655	-154.064746	-154.503455	-

Table 6a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Dimethyl ether [C_2H_6O] Based on Several Levels of Calculation. (CONTINUED)

H5 H4

H6 C1 O2 C3 H8

H7 H9

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
frequencies (cm^{-1})					
ν_1	230	245	215	221	
ν_2	251	253	265	268	
ν_3	421	409	444	427	
ν_4	963	877	1045	972	
ν_5	1190	1090	1234	1152	
ν_6	1253	1172	1281	1193	
ν_7	1281	1176	1316	1228	
ν_8	1283	1204	1350	1236	
ν_9	1361	1270	1402	1299	
ν_{10}	1607	1516	1612	1510	
ν_{11}	1652	1559	1639	1545	
ν_{12}	1672	1589	1650	1547	
ν_{13}	1681	1597	1651	1558	
ν_{14}	1685	1608	1652	1565	
ν_{15}	1700	1621	1671	1582	
ν_{16}	3173	3043	3164	3050	
ν_{17}	3186	3052	3180	3059	
ν_{18}	3230	3106	3216	3117	
ν_{19}	3233	3110	3218	3122	
ν_{20}	3253	3135	3303	3216	
ν_{21}	3264	3146	3305	3217	

Table 6b. Force Constant Matrix for Dimethyl ether [C_2H_6O] at the 6-31G* HF Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.709512D+00				
2	0.199707D-05	0.641971D+00			
3	0.191528D-01	0.000000D+00	0.580925D+00		
4	-0.113569D+00	0.000000D+00	-0.143067D-01	0.464369D+00	
5	0.000000D+00	-0.775614D-01	0.148421D-05	0.000000D+00	0.115487D+00
6	0.342363D-01	0.000000D+00	-0.306053D+00	0.103825D+00	-0.123891D-05
7	-0.446085D-02	0.000000D+00	-0.169505D-01	-0.282047D+00	0.000000D+00
8	0.000000D+00	-0.222050D-02	0.000000D+00	0.000000D+00	-0.775613D-01
9	-0.509398D-01	0.000000D+00	-0.344166D-01	-0.401025D-01	0.000000D+00
10	0.631439D-03	-0.123383D-02	0.735867D-02	-0.399117D-01	-0.321324D-01
11	0.688850D-03	0.404019D-03	0.161334D-02	-0.545827D-02	0.926899D-02
12	-0.147845D-02	-0.342503D-02	0.388477D-02	-0.154699D-01	-0.150938D-01
13	-0.337512D+00	-0.178320D-04	-0.797927D-01	0.505963D-02	0.000000D+00
14	-0.180442D-04	-0.646963D-01	-0.540836D-05	0.000000D+00	0.128006D-02
15	-0.642815D-01	-0.455108D-05	-0.775708D-01	-0.482858D-01	-0.205223D-05
16	-0.124386D+00	0.101751D+00	0.384720D-01	0.384835D-02	-0.837868D-03
17	0.101616D+00	-0.249281D+00	-0.702594D-01	-0.190996D-02	0.926846D-02
18	0.343071D-01	-0.657569D-01	-0.868022D-01	0.177124D-01	-0.354891D-01
19	-0.124359D+00	-0.101735D+00	0.384618D-01	0.384851D-02	0.837927D-03
20	-0.101601D+00	-0.249308D+00	0.702639D-01	0.190954D-02	0.926944D-02
21	0.342983D-01	0.657613D-01	-0.868008D-01	0.177081D-01	0.354917D-01
22	0.631397D-03	0.123384D-02	0.735900D-02	-0.399116D-01	0.321314D-01
23	-0.688877D-03	0.403855D-03	-0.161346D-02	0.545789D-02	0.926895D-02
24	-0.147901D-02	0.342512D-02	0.388493D-02	-0.154694D-01	0.150934D-01
25	-0.648859D-02	0.000000D+00	0.245642D-03	-0.168536D-02	0.000000D+00
26	0.000000D+00	0.288413D-03	0.000000D+00	0.000000D+00	0.128003D-02
27	-0.381571D-02	0.000000D+00	0.294780D-02	-0.561086D-02	0.000000D+00

	6	7	8	9	10
6	0.555989D+00				
7	-0.886457D-01	0.587735D+00			
8	0.000000D+00	0.000000D+00	0.641970D+00		
9	-0.137577D+00	-0.345789D-01	0.000000D+00	0.702704D+00	
10	-0.159858D-02	-0.119798D+00	-0.101234D+00	0.363186D-01	0.145872D+00
11	-0.449566D-02	-0.105299D+00	-0.249297D+00	0.645964D-01	0.122997D+00
12	0.483722D-02	0.404828D-01	0.665371D-01	-0.913725D-01	-0.367806D-01
13	-0.263465D-02	0.272855D-02	0.000000D+00	0.251212D-03	0.152567D-03
14	0.000000D+00	0.000000D+00	0.288419D-03	0.000000D+00	0.482268D-03
15	-0.254664D-01	0.431256D-02	0.000000D+00	-0.626940D-02	-0.397884D-03
16	0.383914D-02	0.118296D-02	-0.263557D-02	-0.123570D-02	0.873309D-04
17	-0.680806D-02	0.119802D-02	0.403999D-03	0.128159D-02	-0.135022D-04
18	-0.389227D-01	0.760233D-02	-0.251148D-02	0.333340D-02	-0.106973D-02
19	0.383870D-02	0.118295D-02	0.263545D-02	-0.123502D-02	0.977037D-03
20	0.680868D-02	-0.119798D-02	0.403866D-03	-0.128149D-02	0.113269D-02
21	-0.389231D-01	0.760210D-02	0.251152D-02	0.333324D-02	-0.144236D-02
22	-0.159803D-02	-0.119802D+00	0.101235D+00	0.363214D-01	0.124132D-01
23	0.449575D-02	0.105301D+00	-0.249291D+00	-0.645988D-01	0.143487D-01
24	0.483699D-02	0.404858D-01	-0.665394D-01	-0.913748D-01	-0.520429D-02
25	-0.512619D-01	-0.667205D-01	0.000000D+00	0.552007D-01	-0.423718D-03
26	0.000000D+00	0.000000D+00	-0.646964D-01	0.337980D-05	-0.434619D-02
27	-0.187214D-01	0.396896D-01	0.319139D-05	-0.348361D+00	0.281609D-02

	11	12	13	14	15
11	0.262726D+00				
12	-0.707588D-01	0.845383D-01			
13	0.113145D-03	0.162917D-03	0.357259D+00		
14	0.341312D-03	0.173425D-03	0.195972D-04	0.570565D-01	
15	-0.489242D-03	0.482320D-04	0.883020D-01	0.550003D-05	0.985961D-01
16	0.992402D-04	0.550457D-04	-0.138799D-01	0.311371D-01	0.114827D-01
17	-0.414793D-03	0.102458D-03	-0.249919D-03	0.243326D-02	0.154178D-02
18	0.290258D-04	-0.360342D-03	-0.312098D-02	0.898876D-02	0.588540D-02

Table 6b. Force Constant Matrix for Dimethyl ether [C_2H_6O] at the 6-31G* HF Level of Calculation. (CONTINUED 1)

19	-0.3021940-03	0.8136470-03	-0.1387600-01	-0.3113940-01	0.1148270-01
20	0.1164630-03	0.8300370-03	0.2477530-03	0.2429140-02	-0.1540230-02
21	-0.1371330-02	0.6997550-03	-0.3119800-02	-0.8989090-02	0.5885420-02
22	-0.1434800-01	-0.5204510-02	0.1526060-03	-0.4822700-03	-0.3977740-03
23	-0.2557550-01	-0.1048250-01	-0.1132100-03	0.3413660-03	0.4892540-03
24	0.1048170-01	0.5293120-02	0.1629000-03	-0.1733530-03	0.4831190-04
25	0.1510130-02	0.1741900-01	-0.8517560-04	0.0000000+00	-0.2216990-02
26	0.2430840-02	0.3211730-01	0.0000000+00	0.5263060-03	0.0000000+00
27	0.3945610-03	-0.7568570-02	-0.2108530-03	0.0000000+00	-0.1156430-02

	16	17	18	19	20
16	0.1217200+00				
17	-0.1144000+00	0.2627070+00			
18	-0.4745230-01	0.8396180-01	0.1087090+00		
19	0.1029770-01	0.1538470-01	-0.6138390-02	0.1216900+00	
20	-0.1537990-01	-0.2557540-01	0.8895330-02	0.1143820+00	0.2627380+00
21	-0.6137240-02	-0.8896270-02	0.7408600-02	-0.4744120-01	-0.8396770-01
22	0.9772280-03	-0.1132630-02	-0.1442390-02	0.8735050-04	0.1349010-04
23	0.3020650-03	0.1165330-03	0.1371340-02	-0.9921340-04	-0.4147110-03
24	0.8136820-03	-0.8299730-03	0.6997020-03	0.5510740-04	-0.1025430-03
25	0.1520710-03	-0.4933260-03	-0.3980370-03	0.1519970-03	0.4932720-03
26	-0.3611980-04	0.3413290-03	0.5112170-03	0.3597790-04	0.3413460-03
27	0.1626620-03	-0.9391960-04	0.4887750-04	0.1626700-03	0.9399470-04

	21	22	23	24	25
21	0.1087080+00				
22	-0.1069730-02	0.1458760+00			
23	-0.2903400-04	-0.1229970+00	0.2627190+00		
24	-0.3603820-03	-0.3678420-01	0.7076180-01	0.8454130-01	
25	-0.3981210-03	-0.4237520-03	-0.1510490-02	0.1741940-01	0.7552300-01
26	-0.5112260-03	0.4346090-02	0.2431530-02	-0.3211670-01	0.0000000+00
27	0.4876540-04	0.2816190-02	-0.3943090-03	-0.7569240-02	-0.3600980-01

	26	27
26	0.5705660-01	
27	-0.3542770-05	0.3803310+00

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.4329500+00				
2	0.1564460-02	0.4329530+00			
3	-0.9827800-03	0.1970440-01	0.3630950+00		
4	0.1210330-01	-0.2175180-02	0.6567760-04	0.3845060+00	
5	0.1970360-01	-0.9829310-03	0.5109030-03	0.4193760-02	0.3630950+00
6	0.1970450-01	-0.9828860-03	0.1143090-02	0.4193880-02	0.5346220-02
7	-0.9830390-03	0.1970390-01	0.5346250-02	0.6565770-04	0.1143210-02
8	-0.2175200-02	0.1210330-01	0.4193860-02	0.4674350-03	0.6562750-04
9	0.4669100-01	0.4669120-01	-0.3181400-02	0.5863190-02	-0.3182530-02
10	-0.1201900-01	0.6188290-01	-0.7674450-02	-0.2550750-03	0.5478770-03
11	0.6245790-01	0.5208170-02	0.1279100-02	-0.5406420-02	-0.6649130-02
12	0.6188190-01	-0.1201980-01	0.5478520-03	-0.6028810-02	-0.7674700-02
13	0.6188270-01	-0.1201900-01	0.3606610-02	-0.6028850-02	-0.8096040-02
14	-0.1201970-01	0.6188210-01	-0.8095930-02	-0.2550690-03	0.3606620-02
15	0.5208110-02	0.6245740-01	-0.6649100-02	0.1651210-02	0.1279100-02
16	-0.3321720-02	-0.1104670-03	0.1259740-02	-0.2047250-03	0.1628850-03
17	0.0000000+00	0.0000000+00	0.9357850-03	0.0000000+00	0.1739440-01
18	-0.1094760-03	-0.3321550-02	0.1628830-03	-0.1604680-01	0.1259430-02
19	0.1110400-03	0.3321880-02	-0.3587000-03	0.1604720-01	-0.1905640-01
20	0.3321700-02	0.1100500-03	-0.1905640-01	0.2047050-03	-0.3586330-03
21	0.0000000+00	0.0000000+00	0.1739470-01	0.0000000+00	0.9358900-03

	6	7	8	9	10
6	0.3630960+00				
7	0.5108540-03	0.3630950+00			
8	0.6571420-04	0.4193850-02	0.3845050+00		
9	-0.3181130-02	-0.3182260-02	0.5863160-02	0.2896340+00	
10	0.3606520-02	-0.8095980-02	-0.6028850-02	-0.5694350-02	0.3057140+00
11	-0.6649120-02	0.1279050-02	0.1651220-02	0.2747160-01	0.7287110-03
12	-0.8095910-02	0.3606560-02	-0.2551340-03	-0.5693440-02	0.4274700-02
13	-0.7674690-02	0.5478860-03	-0.2550020-03	-0.5694310-02	-0.1522850-02
14	0.5478560-03	-0.7674920-02	-0.6028910-02	-0.5693330-02	0.4584380-01

Table 6b. Force Constant Matrix for Dimethyl ether [C_2H_6O] at the 6-31G* HF Level of Calculation. (CONTINUED 2)

15	0.1279060-02	-0.6649200-02	-0.5406550-02	0.2747160-01	0.3500740-01
16	0.3585680-03	0.1905650-01	-0.1604710-01	0.1997160-02	-0.1918250-02
17	-0.1739480-01	-0.9359400-03	0.0000000+00	0.1281530-05	0.1443290-02
18	0.1905630-01	0.3585110-03	-0.2047250-03	0.1999240-02	-0.5690840-03
19	-0.1259950-02	-0.1627860-03	0.2047090-03	-0.1996740-02	0.1957180-02
20	-0.1627880-03	-0.1259650-02	0.1604700-01	-0.1998870-02	0.5655410-01
21	-0.9358220-03	-0.1739460-01	0.0000000+00	0.0000000+00	-0.5280500-01

	11	12	13	14	15
11	0.2979250+00				
12	0.3500740-01	0.3057130+00			
13	0.3500740-01	0.4584400-01	0.3057130+00		
14	0.7281020-03	-0.1522780-02	0.4274840-02	0.3057130+00	
15	0.9128840-02	0.7281960-03	0.7286800-03	0.3500790-01	0.2979240+00
16	0.3846210-03	-0.5692810-03	-0.1957190-02	-0.5655430-01	0.5462540-01
17	0.1142870-05	-0.5280500-01	0.5280480-01	-0.1443150-02	0.0000000+00
18	0.5462560-01	-0.1917740-02	-0.5655420-01	-0.1956910-02	0.3846580-03
19	-0.5462510-01	0.5655420-01	0.1918580-02	0.5692770-03	-0.3845550-03
20	-0.3845870-03	0.1956910-02	0.5690880-03	0.1917800-02	-0.5462550-01
21	0.0000000+00	0.1443190-02	-0.1443260-02	0.5280510-01	0.0000000+00

	16	17	18	19	20
16	0.2120330+00				
17	0.5064920-03	0.2163530+00			
18	0.1237900-04	-0.1056390+00	0.2120330+00		
19	-0.7391240-04	-0.1056400+00	-0.9937430-01	0.2120330+00	
20	-0.9937460-01	0.5064690-03	-0.7405240-04	0.1204830-04	0.2120320+00
21	-0.1056400+00	-0.1995700-02	0.5063250-03	0.5066520-03	-0.1056390+00

	21
21	0.2163530+00

Table 6c. Force Constant Matrix for Dimethyl ether [C_2H_6O] at the 6-31G* MP2 Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.658411D+00				
2	0.364051D-05	0.594951D+00			
3	0.170768D-01	-0.144234D-05	0.500924D+00		
4	-0.930678D-01	0.0000000+00	-0.193805D-01	0.397852D+00	
5	0.0000000+00	-0.687267D-01	0.0000000+00	0.0000000+00	0.102381D+00
6	0.308620D-01	0.0000000+00	-0.254763D+00	0.843403D-01	0.0000000+00
7	-0.112692D-01	0.0000000+00	-0.108382D-01	-0.2377600+00	0.0000000+00
8	0.0000000+00	-0.320875D-02	0.0000000+00	0.0000000+00	-0.6872600-01
9	-0.474642D-01	0.0000000+00	-0.337093D-01	-0.248289D-01	0.0000000+00
10	0.5947090-03	-0.7951060-03	0.734535D-02	-0.358035D-01	-0.2859190-01
11	0.107582D-02	0.117983D-02	0.9031490-03	-0.437913D-02	0.852444D-02
12	-0.214435D-02	-0.368751D-02	0.4015400-02	-0.1159560-01	-0.115107D-01
13	-0.321981D+00	-0.1384300-04	-0.735814D-01	0.380125D-02	0.0000000+00
14	-0.139613D-04	-0.571011D-01	-0.389749D-05	0.0000000+00	0.4870940-03
15	-0.612047D-01	-0.336797D-05	-0.6736960-01	-0.4056780-01	-0.1329750-05
16	-0.113536D+00	0.969721D-01	0.3663880-01	0.2570280-02	-0.4722250-03
17	0.9736900-01	-0.234303D+00	-0.664862D-01	-0.1535390-02	0.8524060-02
18	0.342635D-01	-0.642257D-01	-0.7734190-01	0.1396230-01	-0.3081700-01
19	-0.113517D+00	-0.969617D-01	0.3663230-01	0.2570340-02	0.4723430-03
20	-0.9735860-01	-0.234324D+00	0.6649120-01	0.1535150-02	0.8524860-02
21	0.342577D-01	0.642307D-01	-0.7734160-01	0.1395940-01	0.3081860-01
22	0.594564D-03	0.795165D-03	0.734551D-02	-0.358032D-01	0.285917D-01
23	-0.107586D-02	0.117965D-02	-0.9032000-03	0.4379000-02	0.8524610-02
24	-0.214478D-02	0.3687600-02	0.4015540-02	-0.1159530-01	0.1151060-01
25	-0.623062D-02	0.0000000+00	-0.1238790-02	-0.4359110-02	0.0000000+00
26	0.0000000+00	0.3534080-03	0.0000000+00	0.0000000+00	0.4870960-03
27	-0.3501990-02	0.0000000+00	0.1571160-02	-0.4293830-02	0.0000000+00

	6	7	8	9	10
6	0.462761D+00				
7	-0.750717D-01	0.509805D+00			
8	0.0000000+00	-0.191685D-05	0.594945D+00		
9	-0.110084D+00	-0.401181D-01	0.2692090-05	0.649541D+00	
10	-0.808381D-03	-0.105777D+00	-0.947702D-01	0.372435D-01	0.1291160+00
11	-0.333056D-02	-0.970226D-01	-0.2343090+00	0.6698290-01	0.1122560+00
12	0.348126D-02	0.3961860-01	0.6742460-01	-0.8509220-01	-0.383607D-01
13	-0.115273D-02	0.2153690-02	0.0000000+00	-0.2749580-03	0.2095440-03
14	0.0000000+00	0.0000000+00	0.3533930-03	0.0000000+00	0.4572590-03
15	-0.216263D-01	0.1988240-02	0.0000000+00	-0.6813380-02	-0.1887240-03
16	0.317426D-02	0.1830660-02	-0.3155890-02	-0.1669000-02	0.4150730-04
17	-0.528266D-02	0.4563760-03	0.1179770-02	0.1328470-02	0.6301440-04
18	-0.348921D-01	0.7821270-02	-0.2066670-02	0.2779600-02	-0.9294860-03
19	0.317407D-02	0.1830620-02	0.3155730-02	-0.1668620-02	0.8475080-03
20	0.528288D-02	-0.4563980-03	0.1179660-02	-0.1328400-02	0.1013380-02
21	-0.348924D-01	0.7821190-02	0.2066720-02	0.2779490-02	-0.1509670-02
22	-0.809017D-03	-0.105777D+00	0.9477180-01	0.372425D-01	0.1031510-01
23	0.333052D-02	0.9702410-01	-0.2343120+00	-0.6698150-01	0.1312050-01
24	0.348067D-02	0.3961750-01	-0.6742320-01	-0.8509040-01	-0.4278900-02
25	-0.437088D-01	-0.5503740-01	0.0000000+00	0.4153790-01	0.4555680-03
26	0.0000000+00	0.0000000+00	-0.571011D-01	-0.3712940-05	-0.2752890-02
27	-0.1346550-01	0.2916120-01	-0.3603800-05	-0.3343110+00	0.1487050-02

	11	12	13	14	15
11	0.245715D+00				
12	-0.720670D-01	0.796039D-01			
13	0.186081D-03	0.170553D-03	0.339250D+00		
14	0.298130D-03	0.127756D-03	0.149597D-04	0.511597D-01	
15	-0.360299D-03	0.425450D-04	0.812052D-01	0.397763D-05	0.863969D-01
16	0.989753D-04	0.124262D-03	-0.118223D-01	0.279845D-01	0.105627D-01

Table 6c. Force Constant Matrix for Dimethyl ether [C_2H_6O] at the 6-31G* MP2 Level of Calculation. (CONTINUED 1)

17	-0.567923D-03	0.130260D-03	-0.189267D-02	0.196533D-02	0.103865D-02
18	0.105611D-03	-0.268382D-03	-0.323856D-02	0.782140D-02	0.509335D-02
19	-0.742968D-03	0.117812D-02	-0.118197D-01	-0.279860D-01	0.105627D-01
20	-0.378800D-03	0.118609D-02	0.189129D-02	0.196265D-02	-0.103755D-02
21	-0.137177D-02	0.720056D-03	-0.323778D-02	-0.782172D-02	0.509339D-02
22	-0.131206D-01	-0.427874D-02	0.209553D-03	-0.457234D-03	-0.188656D-03
23	-0.224255D-01	-0.105304D-01	-0.186111D-03	0.298169D-03	0.360298D-03
24	0.105308D-01	0.468122D-02	0.170532D-03	-0.127737D-03	0.425823D-04
25	0.164849D-02	0.152880D-01	-0.118025D-05	0.000000D+00	-0.216888D-02
26	0.196417D-02	0.289270D-01	0.000000D+00	0.576686D-03	0.000000D+00
27	-0.139282D-02	-0.718374D-02	-0.608295D-04	0.000000D+00	-0.859383D-03

	16	17	18	19	20
16	0.111721D+00				
17	-0.107586D+00	0.245707D+00			
18	-0.450633D-01	0.788760D-01	0.970081D-01		
19	0.827692D-02	0.145423D-01	-0.506375D-02	0.111699D+00	
20	-0.145391D-01	-0.224252D-01	0.846204D-02	0.107574D+00	0.245731D+00
21	-0.506288D-02	-0.846261D-02	0.671939D-02	-0.450561D-01	-0.788817D-01
22	0.847634D-03	-0.101331D-02	-0.150968D-02	0.415317D-04	-0.630271D-04
23	0.742910D-03	-0.378758D-03	0.137179D-02	-0.989653D-04	-0.567843D-03
24	0.117820D-02	-0.118610D-02	0.719968D-03	0.124331D-03	-0.130344D-03
25	0.702071D-04	-0.403116D-03	-0.242330D-03	0.701650D-04	0.403072D-03
26	-0.450616D-04	0.298129D-03	0.472624D-03	0.449553D-04	0.298154D-03
27	0.116901D-03	0.442723D-04	0.181944D-03	0.116919D-03	-0.442292D-04

	21	22	23	24	25
21	0.970082D-01				
22	-0.929515D-03	0.129116D+00			
23	-0.105621D-03	-0.112257D+00	0.245718D+00		
24	-0.268412D-03	-0.383593D-01	0.720653D-01	0.796017D-01	
25	-0.242367D-03	0.455574D-03	-0.164836D-02	0.152877D-01	0.645768D-01
26	-0.472626D-03	0.275273D-02	0.196379D-02	-0.289269D-01	0.000000D+00
27	0.181883D-03	0.148690D-02	0.139279D-02	-0.718286D-02	-0.245123D-01

	26	27
26	0.511597D-01	
27	0.371561D-05	0.361068D+00

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.371043D+00				
2	-0.257903D-02	0.371056D+00			
3	-0.472151D-03	0.168844D-01	0.339405D+00		
4	0.958533D-02	-0.135514D-02	-0.816199D-04	0.363057D+00	
5	0.168834D-01	-0.472154D-03	0.520389D-03	0.193725D-02	0.339406D+00
6	0.168839D-01	-0.472282D-03	0.410196D-03	0.193732D-02	0.329786D-02
7	-0.472305D-03	0.168841D-01	0.329802D-02	-0.816187D-04	0.410208D-03
8	-0.135523D-02	0.958551D-02	0.193743D-02	0.261258D-03	-0.816423D-04
9	0.508761D-01	0.508767D-01	-0.245982D-02	0.580945D-02	-0.246030D-02
10	-0.130586D-01	0.564788D-01	-0.933551D-02	-0.377638D-03	0.255816D-03
11	0.569225D-01	0.783976D-02	0.913068D-03	-0.575808D-02	-0.574452D-02
12	0.564776D-01	-0.130592D-01	0.255813D-03	-0.519644D-02	-0.933556D-02
13	0.564780D-01	-0.130587D-01	0.432447D-02	-0.519653D-02	-0.738681D-02
14	-0.130589D-01	0.564787D-01	-0.738673D-02	-0.377584D-03	0.432445D-02
15	0.783969D-02	0.569217D-01	-0.574464D-02	0.134353D-02	0.913078D-03
16	-0.355412D-02	-0.231935D-03	0.159329D-02	-0.257445D-03	0.332975D-03
17	0.000000D+00	0.000000D+00	0.858644D-03	0.000000D+00	0.163475D-01
18	-0.231422D-03	-0.355402D-02	0.332954D-03	-0.153235D-01	0.159320D-02
19	0.232613D-03	0.355431D-02	-0.741909D-03	0.153238D-01	-0.184370D-01
20	0.355417D-02	0.232028D-03	-0.184371D-01	0.257419D-03	-0.741868D-03
21	0.000000D+00	0.000000D+00	0.163478D-01	0.000000D+00	0.858681D-03

	6	7	8	9	10
6	0.339410D+00				
7	0.520361D-03	0.339406D+00			
8	-0.815748D-04	0.193725D-02	0.363055D+00		
9	-0.245956D-02	-0.246006D-02	0.580939D-02	0.284927D+00	
10	0.432432D-02	-0.738675D-02	-0.519662D-02	-0.477470D-02	0.272110D+00
11	-0.574452D-02	0.913016D-03	0.134357D-02	0.264324D-01	0.305351D-03
12	-0.738667D-02	0.432445D-02	-0.377657D-03	-0.477426D-02	0.403786D-02

Table 6c. Force Constant Matrix for Dimethyl ether [C_2H_6O] at the 6-31G* MP2 Level of Calculation. (CONTINUED 2)

13	-0.933584D-02	0.255834D-03	-0.377555D-03	-0.477475D-02	-0.160811D-02
14	0.255813D-03	-0.933565D-02	-0.519656D-02	-0.477369D-02	0.433543D-01
15	0.913019D-03	-0.574454D-02	-0.575817D-02	0.264322D-01	0.314440D-01
16	0.741672D-03	0.184371D-01	-0.153238D-01	0.187802D-02	-0.427095D-02
17	-0.163477D-01	-0.858741D-03	0.000000D+00	0.000000D+00	0.137899D-02
18	0.184368D-01	0.741684D-03	-0.257443D-03	0.187915D-02	-0.808889D-03
19	-0.159363D-02	-0.332849D-03	0.257427D-03	-0.187763D-02	0.227839D-02
20	-0.332844D-03	-0.159370D-02	0.153236D-01	-0.187899D-02	0.519953D-01
21	-0.858658D-03	-0.163475D-01	0.000000D+00	0.000000D+00	-0.477891D-01
	11	12	13	14	15
11	0.265833D+00				
12	0.314435D-01	0.272108D+00			
13	0.314437D-01	0.433546D-01	0.272107D+00		
14	0.304980D-03	-0.160806D-02	0.403804D-02	0.272109D+00	
15	0.903770D-02	0.305161D-03	0.305378D-03	0.314439D-01	0.265833D+00
16	0.505048D-03	-0.809056D-03	-0.227836D-02	-0.519950D-01	0.500583D-01
17	0.113153D-05	-0.477887D-01	0.477887D-01	-0.137889D-02	0.000000D+00
18	0.500583D-01	-0.427095D-02	-0.519951D-01	-0.227814D-02	0.505074D-03
19	-0.500580D-01	0.519952D-01	0.427124D-02	0.809052D-03	-0.504977D-03
20	-0.504975D-03	0.227825D-02	0.808899D-03	0.427035D-02	-0.500583D-01
21	0.000000D+00	0.137897D-02	-0.137902D-02	0.477891D-01	0.000000D+00
	16	17	18	19	20
16	0.194284D+00				
17	0.406594D-03	0.198948D+00			
18	-0.944210D-04	-0.967049D-01	0.194283D+00		
19	0.228682D-03	-0.967048D-01	-0.899965D-01	0.194282D+00	
20	-0.899976D-01	0.406690D-03	0.228604D-03	-0.948471D-04	0.194282D+00
21	-0.967052D-01	-0.224257D-02	0.406523D-03	0.406833D-03	-0.967032D-01
	21				
21	0.198946D+00				

Table 6d. Force Constant Scaling Constants, Q(I), and C matrix for Dimethyl ether [C_2H_6O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation.

Q Values

I	Q(I)
1	0.857010E+00
2	0.857037E+00
3	0.934753E+00
4	0.944215E+00
5	0.934758E+00
6	0.934767E+00
7	0.934760E+00
8	0.944213E+00
9	0.983751E+00
10	0.890081E+00
11	0.892283E+00
12	0.890075E+00
13	0.890074E+00
14	0.890081E+00
15	0.892284E+00
16	0.916289E+00
17	0.919550E+00
18	0.916286E+00
19	0.916282E+00
20	0.916282E+00
21	0.919546E+00

C Matrix (21,21)

		COLUMN 1	COLUMN 2	COLUMN 3
ROW	1	0.1000000000000D+01		
ROW	2	-0.1923535860450+01	0.1000000000000D+01	
ROW	3	0.1000000000000+01	0.9573534563660+00	0.1000000000000+01
ROW	4	0.8803896673690+00	0.6925565915220+00	0.1000000000000D+01
ROW	5	0.9573552881250+00	0.1000000000000+01	0.1000000000000+01
ROW	6	0.9573310629810+00	0.1000000000000+01	0.3838927685350+00
ROW	7	0.1000000000000+01	0.9573654139670+00	0.6599410240710+00
ROW	8	0.6926056927590+00	0.8803944128120+00	0.4917329533170+00
ROW	9	0.1186709915600+01	0.1186701142730+01	0.8062958899800+00
ROW	10	0.1244009725200+01	0.1044960922660+01	0.1333606428490+01
ROW	11	0.1042203035170+01	0.1721338286430+01	0.7816276922220+00
ROW	12	0.1044975786460+01	0.1243956177600+01	0.1000000000000+01
ROW	13	0.1044969645740+01	0.1243990187210+01	0.1314533983420+01
ROW	14	0.1243953763740+01	0.1044973463750+01	0.1000281077300+01
ROW	15	0.1721369213080+01	0.1042180805750+01	0.9460175896100+00
ROW	16	0.1207424925780+01	0.1000000000000+01	0.1366616450890+01
ROW	17	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	18	0.1000000000000+01	0.1207434684730+01	0.1000000000000+01
ROW	19	0.1000000000000+01	0.1207415747190+01	0.1000000000000+01
ROW	20	0.1207453926760+01	0.1000000000000+01	0.1045418682310+01
ROW	21	0.1000000000000+01	0.1000000000000+01	0.1013695234540+01

		COLUMN 4	COLUMN 5	COLUMN 6
ROW	4	0.1000000000000+01		
ROW	5	0.4916972806030+00	0.1000000000000+01	
ROW	6	0.4916970590130+00	0.6599079584250+00	0.1000000000000+01
ROW	7	0.1000000000000+01	0.3838659553780+00	0.1000000000000+01
ROW	8	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01

Table 6d. Force Constant Scaling Constants, Q(I), and C matrix for Dimethyl ether [C_2H_6O] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED)

ROW	9	0.1028070327160+01	0.8061652301140+00	0.8062709927560+00
ROW	10	0.1000000000000+01	0.1000000000000+01	0.1314505020570+01
ROW	11	0.1160327492100+01	0.9459931812820+00	0.9459911685790+00
ROW	12	0.9402109750720+00	0.1333570909000+01	0.1000271547750+01
ROW	13	0.9402222570980+00	0.1000280296300+01	0.1333607086590+01
ROW	14	0.1000000000000+01	0.1314518909200+01	0.1000000000000+01
ROW	15	0.8864583526320+00	0.7816325290290+00	0.7816025747340+00
ROW	16	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	17	0.1000000000000+01	0.1013686852930+01	0.1013671175320+01
ROW	18	0.1026642812120+01	0.1366882874620+01	0.1045393543230+01
ROW	19	0.1026640355410+01	0.1045403989080+01	0.1366689075190+01
ROW	20	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	21	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 7	COLUMN 8	COLUMN 9
ROW	7	0.1000000000000+01		
ROW	8	0.4916864897910+00	0.1000000000000+01	
ROW	9	0.8061533278300+00	0.1028065983490+01	0.1000000000000+01
ROW	10	0.1000273782060+01	0.9402363010730+00	0.8960763858720+00
ROW	11	0.7816073657870+00	0.8864825761010+00	0.1026972014640+01
ROW	12	0.1314541652220+01	0.1000000000000+01	0.8961405546250+00
ROW	13	0.1000000000000+01	0.1000000000000+01	0.8960939852950+00
ROW	14	0.1333539597470+01	0.9402159994250+00	0.8960462133980+00
ROW	15	0.9459851697040+00	0.1160317847820+01	0.1026962440950+01
ROW	16	0.1045402467480+01	0.1026642793150+01	0.9904373653000+00
ROW	17	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	18	0.1000000000000+01	0.1000000000000+01	0.9900078819830+00
ROW	19	0.1000000000000+01	0.1000000000000+01	0.9904443802520+00
ROW	20	0.1367081607670+01	0.1026637016360+01	0.9901059628450+00
ROW	21	0.1013675466800+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 10	COLUMN 11	COLUMN 12
ROW	10	0.1000000000000+01		
ROW	11	0.1000000000000+01	0.1000000000000+01	
ROW	12	0.1061248511590+01	0.1007873893340+01	0.1000000000000+01
ROW	13	0.1186401560190+01	0.1007880249800+01	0.1062494117070+01
ROW	14	0.1062481959360+01	0.1000000000000+01	0.1186412558320+01
ROW	15	0.1007886751290+01	0.1109531190660+01	0.1000000000000+01
ROW	16	0.2465398338030+01	0.1000000000000+01	0.1000000000000+01
ROW	17	0.1056103459220+01	0.1000000000000+01	0.1000343667900+01
ROW	18	0.1000000000000+01	0.1013475285510+01	0.2466076814310+01
ROW	19	0.1289045012320+01	0.1013481178930+01	0.1018053507610+01
ROW	20	0.1018052233060+01	0.1000000000000+01	0.1289151693800+01
ROW	21	0.1000351081020+01	0.1000000000000+01	0.1056163660930+01

		COLUMN 13	COLUMN 14	COLUMN 15
ROW	13	0.1000000000000+01		
ROW	14	0.1061263681780+01	0.1000000000000+01	
ROW	15	0.1000000000000+01	0.1007869864150+01	0.1000000000000+01
ROW	16	0.1289018482880+01	0.1018039891550+01	0.1013476849110+01
ROW	17	0.1000347762550+01	0.1056124551240+01	0.1000000000000+01
ROW	18	0.1018049070580+01	0.1289077230220+01	0.1000000000000+01
ROW	19	0.2465164277990+01	0.1000000000000+01	0.1000000000000+01
ROW	20	0.1000000000000+01	0.2465644350880+01	0.1013478404920+01
ROW	21	0.1056148555670+01	0.1000348887370+01	0.1000000000000+01

		COLUMN 16	COLUMN 17	COLUMN 18
ROW	16	0.1000000000000+01		
ROW	17	0.1000000000000+01	0.1000000000000+01	
ROW	18	0.1000000000000+01	0.9972881268800+00	0.1000000000000+01
ROW	19	0.1000000000000+01	0.9972828572230+00	0.9883744591830+00
ROW	20	0.9883812506980+00	0.1000000000000+01	0.1000000000000+01
ROW	21	0.9972860997670+00	0.1222016225820+01	0.1000000000000+01

		COLUMN 19	COLUMN 20	COLUMN 21
ROW	19	0.1000000000000+01		
ROW	20	0.1000000000000+01	0.1000000000000+01	
ROW	21	0.1000000000000+01	0.9972778039640+00	0.1000000000000+01

Table 7a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] Based on Several Levels of Calculation.

H5 H8

H6 C1 O2 C3 O4 H10

H7 H9

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
geometry					
$r(C_1\text{-}O_2)$/A	1.4419	1.4776	1.4009	1.4268	-
$r(O_2\text{-}C_3)$/A	1.4140	1.4486	1.3803	1.4042	-
$r(C_3\text{-}O_4)$/A	1.4214	1.4519	1.3868	1.4112	-
$r(C_1\text{-}H_5)$/A	1.0814	1.0937	1.0808	1.0899	-
$r(C_1\text{-}H_6)$/A	1.0814	1.0937	1.0876	1.0978	-
$r(C_1\text{-}H_7)$/A	1.0814	1.0937	1.0834	1.0932	-
$r(C_3\text{-}H_8)$/A	1.0793	1.0941	1.0840	1.0966	-
$r(C_3\text{-}H_9)$/A	1.0793	1.0941	1.0830	1.0951	-
$r(O_4\text{-}H_{10})$/A	0.9671	0.9932	0.9485	0.9733	-
$\phi(C_3\text{-}O_2\text{-}C_1)$/°	114.6894	110.7483	115.0558	112.1624	-
$\phi(O_4\text{-}C_3\text{-}O_2)$/°	112.4544	113.1792	113.0114	113.2533	-
$\phi(H_5\text{-}C_1\text{-}O_2)$/°	106.5666	105.9106	107.1056	106.3415	-
$\phi(H_6\text{-}C_1\text{-}O_2)$/°	110.8033	111.0440	110.9215	110.7154	-
$\phi(H_7\text{-}C_1\text{-}O_2)$/°	110.8056	110.4249	111.5826	111.4225	-
$\phi(H_8\text{-}C_3\text{-}O_2)$/°	111.5406	111.9870	111.2064	111.4320	-
$\phi(H_9\text{-}C_3\text{-}O_2)$/°	105.5199	104.3135	105.8620	105.0216	-
$\phi(H_{10}\text{-}O_4\text{-}C_3)$/°	110.4560	106.9396	108.8327	106.4759	-
$\tau(O_4\text{-}C_3\text{-}O_2\text{-}C_1)$/°	62.8174	61.8618	67.0973	65.2281	-
$\tau(H_5\text{-}C_1\text{-}O_2\text{-}C_3)$/°	-177.5409	-173.7236	-182.5361	-182.6930	-
$\tau(H_6\text{-}C_1\text{-}O_2\text{-}C_3)$/°	63.3481	67.0267	58.6578	58.5265	-
$\tau(H_7\text{-}C_1\text{-}O_2\text{-}C_3)$/°	-57.6887	-53.8959	-62.8481	-62.9162	-
$\tau(H_8\text{-}C_3\text{-}O_2\text{-}C_1)$/°	-54.9518	-55.4856	-51.7340	-52.8809	-
$\tau(H_9\text{-}C_3\text{-}O_2\text{-}C_1)$/°	-174.7469	-175.2089	-170.7632	-172.3266	-
$\tau(H_{10}\text{-}O_4\text{-}C_3\text{-}O_2)$/°	61.0154	60.7055	61.1461	61.1098	-
E/a.u.	-227.661103	-228.085065	-228.927586	-229.557740	-

Table 7a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] Based on Several Levels of Calculation. (CONTINUED)

H5 H8

H6 C1 O2 C3 O4 H10

H7 H9

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
frequencies (cm^{-1})					
$\tilde{\nu}_1$	151	161	136	132	
ν_2	201	200	214	215	
ν_3	369	356	397	383	
ν_4	421	418	423	416	
ν_5	622	586	645	606	
ν_6	973	887	1040	965	
ν_7	1094	993	1142	1062	
ν_8	1144	1047	1208	1104	
ν_9	1228	1114	1280	1184	
ν_{10}	1267	1182	1299	1208	
ν_{11}	1299	1201	1350	1236	
ν_{12}	1404	1314	1438	1333	
ν_{13}	1498	1419	1521	1419	
ν_{14}	1564	1465	1589	1471	
ν_{15}	1626	1526	1639	1527	
ν_{16}	1671	1587	1645	1551	
ν_{17}	1696	1605	1663	1575	
ν_{18}	1701	1624	1688	1583	
ν_{19}	3208	3079	3196	3083	
ν_{20}	3236	3083	3234	3096	
ν_{21}	3270	3139	3270	3164	
ν_{22}	3283	3152	3283	3175	
ν_{23}	3287	3171	3316	3230	
ν_{24}	3866	3516	4093	3761	

Table 7b. Force Constant Matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] at the 6-31G* HF Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.711882D+00				
2	0.439169D-02	0.657337D+00			
3	0.128360D-01	-0.756100D-02	0.565897D+00		
4	-0.114434D+00	0.152681D-04	-0.555828D-02	0.461147D+00	
5	0.100264D-02	-0.777232D-01	0.133380D-02	-0.771113D-03	0.128865D+00
6	0.338584D-01	-0.126747D-02	-0.286087D+00	0.101780D+00	-0.404661D-02
7	-0.647044D-03	0.761235D-03	-0.287642D-01	-0.264087D+00	0.208143D-01
8	0.195751D-02	0.618848D-03	-0.656318D-02	0.258425D-01	-0.864743D-01
9	-0.503454D-01	-0.632717D-03	-0.351744D-01	-0.417982D-01	0.330700D-02
10	0.717758D-03	0.459574D-03	0.981550D-02	-0.502798D-01	-0.544414D-01
11	-0.527680D-03	-0.144036D-02	0.852681D-02	-0.328191D-01	-0.124642D-02
12	0.955885D-03	0.147922D-02	-0.116220D-02	-0.130950D-01	-0.152072D-01
13	-0.339836D+00	-0.125488D-01	-0.779776D-01	0.525478D-02	0.460253D-03
14	-0.125386D-01	-0.656311D-01	-0.308724D-02	0.805726D-03	0.167404D-02
15	-0.627413D-01	-0.321313D-02	-0.754022D-01	-0.489284D-01	-0.113966D-02
16	-0.132357D+00	0.108060D+00	0.415507D-01	0.374876D-02	-0.109568D-02
17	0.107961D+00	-0.246362D+00	-0.686174D-01	-0.255830D-02	0.839516D-02
18	0.361986D-01	-0.638599D-01	-0.855922D-01	0.180692D-01	-0.344066D-01
19	-0.120253D+00	-0.102886D+00	0.414811D-01	0.550935D-02	0.167001D-02
20	-0.101330D+00	-0.268040D+00	0.793834D-01	0.358215D-02	0.992819D-02
21	0.355611D-01	0.723745D-01	-0.889826D-01	0.153727D-01	0.350155D-01
22	0.849542D-03	0.745823D-03	0.755139D-02	-0.425179D-01	0.264291D-01
23	-0.893995D-03	0.238959D-03	-0.607428D-03	0.421200D-02	0.668299D-02
24	-0.179037D-02	0.325832D-02	0.369122D-02	-0.189861D-01	0.137917D-01
25	-0.558811D-02	0.133980D-02	0.741377D-03	-0.486445D-02	0.323801D-02
26	0.176366D-03	0.137282D-02	-0.878297D-03	0.542368D-03	0.449478D-02
27	-0.397632D-02	0.755708D-03	0.332963D-02	-0.745957D-02	0.145638D-03
28	-0.333260D-03	-0.339117D-03	-0.167599D-02	0.524352D-03	0.269393D-02
29	-0.199633D-03	-0.371403D-03	-0.192946D-02	0.114853D-02	0.540368D-02
30	-0.556555D-03	-0.133356D-02	-0.516566D-03	0.603248D-03	0.120656D-02

	6	7	8	9	10
6	0.547730D+00				
7	-0.790784D-01	0.607039D+00			
8	0.141770D-01	-0.789572D-01	0.662356D+00		
9	-0.158227D+00	-0.625125D-01	0.172412D-01	0.758572D+00	
10	-0.858403D-02	-0.141980D+00	-0.404857D-01	0.438444D-01	0.378499D+00
11	-0.129431D-01	-0.831075D-01	-0.256748D+00	0.488435D-01	-0.787167D-01
12	0.161119D-01	0.366275D-01	0.189640D-01	-0.112550D+00	-0.176954D+00
13	-0.224858D-02	0.233629D-02	-0.813582D-04	0.116802D-02	-0.111154D-03
14	-0.242066D-03	-0.906773D-04	-0.735248D-03	0.752561D-03	-0.115147D-03
15	-0.270321D-01	0.594496D-02	0.712263D-03	-0.637590D-02	-0.979045D-03
16	0.332535D-02	0.125611D-02	-0.276431D-02	-0.181993D-02	-0.115960D-03
17	-0.632324D-02	0.208584D-02	-0.149948D-04	0.130129D-02	-0.890159D-03
18	-0.390928D-01	0.918140D-02	-0.233644D-02	0.331303D-02	-0.176352D-02
19	0.190667D-02	-0.400415D-03	0.124998D-02	-0.437601D-03	-0.156433D-03
20	0.528472D-02	-0.311387D-02	-0.144913D-02	0.273960D-03	0.339875D-03
21	-0.371708D-01	0.782819D-02	0.424220D-02	0.227152D-02	-0.129192D-02
22	0.494462D-03	-0.148592D+00	0.119181D+00	0.627070D-01	0.134483D-01
23	0.142274D-03	0.110536D+00	-0.203243D+00	-0.734031D-01	0.146154D-01
24	0.910410D-02	0.681013D-01	-0.861944D-01	-0.124505D+00	-0.456812D-02
25	-0.521280D-01	-0.699600D-01	0.187372D-02	0.592260D-01	-0.458602D-02
26	0.335079D-02	0.402937D-02	-0.755206D-01	0.235223D-01	-0.205002D-01
27	-0.237350D-01	0.470924D-01	0.316327D-01	-0.333803D+00	0.568522D-02
28	0.673720D-03	0.150351D-01	-0.278162D-01	-0.100319D-01	-0.195436D+00
29	0.186769D-02	0.270421D-01	-0.387894D-01	-0.212059D-01	0.179735D+00
30	-0.160146D-02	-0.442068D-02	0.812470D-02	0.647814D-02	0.134796D+00

	11	12	13	14	15
11	0.666802D+00				
12	0.126779D+00	0.196651D+00			
13	-0.314487D-04	-0.584777D-03	0.359445D+00		
14	0.707455D-03	-0.870476D-03	0.135409D-01	0.576954D-01	

Table 7b. Force Constant Matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] at the 6-31G* HF Level of Calculation. (CONTINUED 1)

15	-0.128555D-02	0.117182D-02	0.859745D-01	0.349943D-02	0.971064D-01
16	0.570583D-03	0.231218D-03	-0.148331D-01	0.305958D-01	0.112545D-01
17	0.217816D-03	-0.571961D-03	-0.110114D-02	0.386577D-02	0.212911D-02
18	-0.598263D-03	0.147747D-03	-0.341433D-02	0.894731D-02	0.569093D-02
19	0.307040D-04	-0.108626D-02	-0.124909D-01	-0.317006D-01	0.117653D-01
20	0.976630D-03	-0.251364D-02	-0.208059D-04	0.176722D-02	-0.139184D-02
21	-0.327262D-02	0.163325D-02	-0.284531D-02	-0.924505D-02	0.605892D-02
22	-0.220388D-01	-0.769319D-02	0.304306D-03	-0.490537D-03	-0.365369D-03
23	-0.426566D-01	-0.158287D-01	-0.167467D-03	0.276356D-03	0.385584D-03
24	0.756836D-02	0.800791D-02	0.758310D-04	-0.878595D-04	0.132508D-03
25	-0.166668D-01	0.206272D-01	-0.108171D-03	-0.403723D-04	-0.195972D-02
26	-0.185743D-01	0.403232D-01	-0.201032D-03	0.288803D-03	0.987796D-04
27	0.815075D-02	0.255300D-02	-0.267266D-03	0.178545D-03	-0.133150D-02
28	0.233307D+00	0.140972D+00	0.385697D-04	0.335441D-04	0.344754D-04
29	-0.348038D+00	-0.152553D+00	0.150939D-03	0.913438D-04	0.205019D-03
30	-0.181769D+00	-0.112564D+00	0.119529D-03	0.154849D-03	-0.189338D-04

	16	17	18	19	20
16	0.130632D+00				
17	-0.121730D+00	0.257914D+00			
18	-0.496169D-01	0.813690D-01	0.107195D+00		
19	0.106676D-01	0.176858D-01	-0.686410D-02	0.116910D+00	
20	-0.138361D-01	-0.245005D-01	0.872319D-02	0.114126D+00	0.281540D+00
21	-0.573632D-02	-0.910719D-02	0.736976D-02	-0.470095D-01	-0.896575D-01
22	0.872560D-03	-0.122639D-02	-0.170449D-02	0.134172D-03	0.135092D-03
23	0.345201D-03	0.118534D-03	0.108578D-02	0.958113D-04	-0.178705D-03
24	0.669114D-03	-0.538102D-03	0.794101D-03	0.350408D-04	-0.155402D-03
25	0.213285D-03	-0.506195D-03	-0.420428D-03	0.000000D+00	0.236573D-03
26	-0.115852D-03	0.346477D-03	0.670766D-03	-0.126803D-03	0.692812D-04
27	0.109574D-03	-0.952539D-04	0.192721D-03	0.151160D-03	0.966094D-04
28	-0.838991D-04	0.278947D-03	0.334545D-03	0.804147D-04	-0.119139D-03
29	-0.301168D-04	0.196617D-04	0.405198D-03	-0.145061D-03	-0.112879D-03
30	0.325955D-04	0.453755D-03	-0.187602D-04	0.581591D-04	-0.434615D-04

	21	22	23	24	25
21	0.110040D+00				
22	-0.921556D-03	0.175402D+00			
23	-0.226560D-04	-0.121849D+00	0.236669D+00		
24	-0.317204D-03	-0.641535D-01	0.853965D-01	0.112282D+00	
25	-0.818243D-03	0.493986D-03	-0.227674D-02	0.201054D-01	0.845738D-01
26	-0.388791D-03	0.398977D-02	0.734630D-02	-0.258065D-01	0.121172D-01
27	-0.186715D-03	0.306895D-02	0.718171D-03	-0.109803D-01	-0.444383D-01
28	-0.139063D-03	-0.394408D-03	-0.461802D-02	0.511394D-03	-0.173821D-03
29	0.616316D-04	-0.487668D-02	-0.525442D-02	0.276743D-02	0.684822D-03
30	-0.715969D-03	0.101629D-02	0.213349D-02	0.179054D-02	-0.935339D-03

	26	27	28	29	30
26	0.774210D-01				
27	-0.421560D-01	0.363538D+00			
28	0.888123D-04	0.341583D-04	0.180743D+00		
29	0.275543D-02	0.573179D-03	-0.203509D+00	0.384296D+00	
30	0.126379D-02	0.422821D-03	-0.130713D+00	0.169808D+00	0.106745D+00

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.418524D+00				
2	0.117719D-01	0.436556D+00			
3	-0.390137D-02	0.503255D-01	0.427780D+00		
4	0.115036D-01	-0.222270D-02	0.299909D-03	0.385681D+00	
5	0.182219D-01	-0.170663D-02	0.548056D-03	0.400414D-02	0.366591D-01
6	0.153864D-01	-0.504253D-02	0.236783D-02	0.396727D-02	0.460575D-02
7	-0.402866D-03	0.177811D-01	0.138607D-01	-0.785502D-04	0.120682D-02
8	-0.241215D-02	0.143016D-01	0.172143D-01	0.495307D-03	0.457123D-04
9	0.724498D-03	-0.503498D-03	0.100847D-02	-0.179690D-03	-0.729537D-04
10	0.520849D-01	0.517682D-01	0.625590D-03	0.538122D-02	-0.288545D-02
11	-0.539052D-02	0.706873D-01	-0.990843D-02	0.570807D-03	0.145273D-02
12	0.642579D-01	0.202996D-02	0.318178D-02	-0.564364D-02	-0.622937D-02
13	0.619548D-01	-0.140032D-01	0.156509D-02	-0.580366D-02	-0.793442D-02
14	0.634688D-01	-0.770915D-02	0.599132D-02	-0.613189D-02	-0.779636D-02
15	-0.127579D-01	0.659502D-01	-0.363887D-01	-0.360895D-03	0.348163D-02

Table 7b. Force Constant Matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] at the 6-31G* HF Level of Calculation. (CONTINUED 2)

16	0.4332500-02	0.7193770-01	-0.3795500-01	0.1601320-02	0.1295260-02
17	0.2579340-02	-0.1631030-02	0.4270480-01	-0.2363000-03	-0.5009020-03
18	0.4785040-03	0.6010490-03	0.4354100-02	0.2038840-03	-0.3759790-03
19	-0.7312590-04	-0.1348050-02	0.1450120-02	-0.1010960-03	0.1718540-01
20	0.1587560-02	-0.2641020-02	-0.4279400-03	-0.1593400-01	0.1189860-02
21	-0.1494330-02	0.1402380-02	-0.1038980-02	0.1630520-01	-0.1940420-01
22	0.1950970-02	0.6209090-03	-0.5611380-01	0.8431120-04	0.2654150-03
23	-0.6426640-04	0.1578470-02	0.5360280-01	-0.3846060-03	0.1182600-02
24	0.2782680-02	0.1780630-02	-0.6010670-03	-0.1636610-03	-0.7754760-03
	6	7	8	9	10
6	0.3780830+00				
7	0.3617840-03	0.3750560+00			
8	0.1082910-03	0.5015440-02	0.3767400+00		
9	-0.2763200-04	-0.2148530-02	0.1421960-03	0.6017670+00	
10	-0.8278410-02	-0.4271350-02	0.5745650-02	0.6713440-03	0.2984020+00
11	-0.4427660-02	-0.5779060-02	-0.2531080-02	-0.7481680-02	0.8169240-02
12	-0.5938990-02	0.1203970-02	0.1850900-02	-0.1665110-03	0.2394590-01
13	-0.7126010-02	0.3592800-02	-0.3647580-03	-0.2279390-03	-0.6578370-02
14	-0.9831230-02	0.5732120-03	-0.9703320-04	0.3922400-03	-0.3376070-03
15	0.7257670-03	-0.4529950-02	-0.8556480-02	-0.2086120-02	-0.4541970-02
16	0.1085740-02	-0.8723880-02	0.2536520-03	0.9020470-03	0.2637770-01
17	-0.3569420-03	0.4700120-02	-0.1062620-03	0.1889460-01	0.6921950-03
18	-0.4215720-02	0.1473910-01	-0.9119880-02	0.1307160-01	0.9560460-02
19	-0.1638140-01	-0.9016980-03	0.2833850-03	0.2103460-03	-0.8710280-03
20	0.1729200-01	0.5900650-03	-0.8247520-04	-0.1076010-03	0.4752600-02
21	0.1819430-03	-0.2414500-03	0.2423150-03	-0.1805330-03	-0.1217490-02
22	0.2014180-03	0.1904280-02	0.1472650-01	-0.6371930-02	-0.4291750-02
23	-0.2791800-03	-0.1478260-01	-0.6382100-02	-0.5102540-02	-0.2376020-02
24	0.3973350-03	0.2646950-04	0.5632840-03	0.2963200-02	0.2413430-02
	11	12	13	14	15
11	0.4927030+00				
12	-0.2143470-02	0.2981540+00			
13	0.3346590-02	0.3332310-01	0.3051390+00		
14	0.9476060-03	0.3515190-01	0.4467000-01	0.3013760+00	
15	0.8200070-01	0.5997400-03	-0.5055650-03	0.3412340-02	0.3247730+00
16	0.7158490-01	0.8371220-02	0.5744230-03	0.2968840-02	0.4384240-01
17	-0.3199810-01	-0.4668610-03	-0.1581230-02	-0.3361080-03	-0.1427420-01
18	-0.8212090-03	-0.4272260-02	-0.1435280-02	0.4932110-02	-0.7014390-01
19	-0.3458050-02	0.1349520-02	-0.5254370-01	0.5242230-01	-0.1405250-02
20	0.2321120-02	0.5399110-01	-0.1157210-02	-0.5473670-01	-0.1399970-02
21	0.1066560-02	-0.5542360-01	0.5750810-01	0.3682680-02	0.5915700-03
22	0.7613030-01	-0.1471050-03	0.1720710-02	0.2356570-03	0.2094000-01
23	-0.6180360-01	0.3978260-03	0.2183870-02	-0.1313850-02	0.4679040-01
24	-0.4121340-02	0.1963650-03	0.2564210-03	0.2272630-02	0.6680200-02
	16	17	18	19	20
16	0.3272770+00				
17	0.2544980-02	0.2035310+00			
18	0.6585970-01	0.2999110-01	0.3430050+00		
19	0.3599990-04	0.1081870-03	-0.9785300-03	0.2175360+00	
20	0.2719920-03	0.1309630-03	-0.3145450-02	-0.1075520+00	0.2097510+00
21	-0.3834490-03	0.6188590-04	0.5645920-03	-0.1058950+00	-0.1005140+00
22	-0.4982410-01	-0.2345050-01	-0.1562940+00	0.2719930-03	-0.1799100-03
23	-0.2065570-01	-0.4977830-02	-0.1673430+00	-0.1243680-02	0.3482190-03
24	-0.3061630-02	-0.7084160-02	0.8544510-02	0.4433040-03	-0.8657600-03
	21	22	23	24	
21	0.2120850+00				
22	0.1813730-03	0.2622080+00			
23	0.4574830-03	-0.9896120-01	0.2738300+00		
24	0.4294160-03	-0.1368410-02	-0.2958910-02	0.1919280-01	

Table 7c. Force Constant Matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] at the 6-31G* MP2 Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.660839D+00				
2	0.4129960-02	0.6099390+00			
3	0.1133800-01	-0.8007730-02	0.485547D+00		
4	-0.935152D-01	0.4031560-03	-0.9831280-02	0.3891020+00	
5	0.100915D-02	-0.6876730-01	0.1783300-02	-0.3157740-02	0.1119300+00
6	0.3048790-01	-0.130097D-02	-0.2350720+00	0.7914590-01	-0.4151140-02
7	-0.749021D-02	0.1156500-02	-0.2296560-01	-0.2164760+00	0.1893260-01
8	0.222732D-02	-0.7019220-03	-0.7072220-02	0.2664530-01	-0.7394930-01
9	-0.472951D-01	-0.4845680-03	-0.3480380-01	-0.2727550-01	0.1127030-02
10	0.9005560-03	0.6572560-03	0.9217890-02	-0.4565450-01	-0.4573850-01
11	-0.149291D-03	0.1899410-03	0.7688560-02	-0.3179750-01	-0.1329660-02
12	0.6279990-04	0.8408600-03	-0.7891990-03	-0.7729450-02	-0.9259500-02
13	-0.324204D+00	-0.1279460-01	-0.7214360-01	0.4022720-02	0.4990470-03
14	-0.127471D-01	-0.5797830-01	-0.3105650-02	0.9060440-03	0.9795290-03
15	-0.5999660-01	-0.3274840-02	-0.6522530-01	-0.4114450-01	-0.8830400-03
16	-0.1219790+00	0.1035630+00	0.3955390-01	0.2474210-02	-0.6312710-03
17	0.104236D+00	-0.2314240+00	-0.6477250-01	-0.2215190-02	0.7391640-02
18	0.3619360-01	-0.6198950-01	-0.7576180-01	0.1412790-01	-0.2992790-01
19	-0.1094400+00	-0.9834930-01	0.4004610-01	0.4283490-02	0.1389290-02
20	-0.9724540-01	-0.2532060+00	0.7554250-01	0.3313870-02	0.9023730-02
21	0.3579930-01	0.7082670-01	-0.7869220-01	0.1154700-01	0.3027570-01
22	0.7872780-03	0.1531820-03	0.7346620-02	-0.3704090-01	0.2385190-01
23	-0.123197D-02	0.7735190-03	0.2628130-03	0.2899220-02	0.5825600-02
24	-0.2507200-02	0.3683940-02	0.3725230-02	-0.1425010-01	0.1032450-01
25	-0.5519810-02	0.1060790-02	-0.9225500-03	-0.7416250-02	0.2019220-02
26	-0.8565420-04	0.1565810-02	-0.6510870-03	0.1373820-02	0.3363660-02
27	-0.3585500-02	0.6591070-03	0.1911360-02	-0.5917230-02	-0.4379260-03
28	-0.3786870-03	0.1973040-04	-0.1639520-02	0.2210610-03	0.1826350-02
29	-0.1434600-03	-0.3906990-03	-0.1667930-02	0.1629070-02	0.5532180-02
30	-0.4971950-03	-0.9530090-03	-0.8390960-03	0.1327200-02	0.1148970-02

	6	7	8	9	10
6	0.451498D+00				
7	-0.6565490-01	0.5026980+00			
8	0.1212060-01	-0.8655660-01	0.581633D+00		
9	-0.1273860+00	-0.5851200-01	0.2679280-01	0.6890980+00	
10	-0.5007330-02	-0.1098870+00	-0.2743800-01	0.3823390-01	0.3053600+00
11	-0.9783790-02	-0.6246690-01	-0.2123640+00	0.4769090-01	-0.6898450-01
12	0.1453960-01	0.3123830-01	0.1656650-01	-0.1002920+00	-0.1554700+00
13	-0.5713860-03	0.1620310-02	-0.2463010-03	0.6569590-03	0.3857570-04
14	0.5806060-04	-0.3406020-03	-0.8244330-03	0.6797540-03	-0.1852280-03
15	-0.2307680-01	0.3722700-02	0.5964610-03	-0.7042640-02	-0.6540360-03
16	0.2601190-02	0.2049420-02	-0.3306090-02	-0.2299710-02	-0.1987500-03
17	-0.4781150-02	0.1333020-02	0.8795330-03	0.1304500-02	-0.7319810-03
18	-0.3478770-01	0.9290380-02	-0.1905250-02	0.2608350-02	-0.1475960-02
19	0.1396810-02	-0.1809730-04	0.1472610-02	-0.7945890-03	-0.4312270-03
20	0.3839470-02	-0.2735180-02	-0.8779830-03	0.3211530-03	0.2956300-03
21	-0.3315760-01	0.8230150-02	0.4094510-02	0.1757480-02	-0.1399620-02
22	0.1089980-02	-0.1261010+00	0.1094720+00	0.5822970-01	0.9703980-02
23	-0.5985500-03	0.1025610+00	-0.1903300+00	-0.7444010-01	0.1075200-01
24	0.6812820-02	0.6163000-01	-0.8442650-01	-0.1136890+00	-0.3325690-02
25	-0.4424510-01	-0.5588460-01	0.4616930-02	0.4600050-01	-0.2769320-02
26	0.3041670-02	0.4927210-02	-0.6433230-01	0.1665420-01	-0.1571420-01
27	-0.1814340-01	0.3599660-01	0.2258200-01	-0.3151540+00	0.4553630-02
28	0.7569480-03	0.9488940-02	-0.2688730-01	-0.6944200-02	-0.1570630+00
29	0.1555790-02	0.2316880-01	-0.3913250-01	-0.1964560-01	0.1470880+00
30	-0.1226750-02	-0.2975600-02	0.1065110-01	0.4903860-02	0.1153280+00

	11	12	13	14	15
11	0.552283D+00				
12	0.1031420+00	0.1795350+00			

Table 7c. Force Constant Matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] at the 6-31G* MP2 Level of Calculation. (CONTINUED 1)

13	0.1492430-03	-0.5620610-03	0.3414490+00		
14	0.6633930-03	-0.9388550-03	0.1382300-01	0.5182810-01	
15	-0.9402840-03	0.1319130-02	0.7906990-01	0.3360510-02	0.8483640-01
16	0.7470820-03	0.4804110-03	-0.1258430-01	0.2751390-01	0.1028850-01
17	-0.2153910-04	-0.4265850-03	-0.2743770-02	0.3268890-02	0.1644170-02
18	-0.4207970-03	0.3291820-03	-0.3479320-02	0.7800290-02	0.4916970-02
19	-0.3372960-03	-0.8224600-03	-0.1070120-01	-0.2857010-01	0.1078710-01
20	0.4827180-03	-0.2203000-02	0.1632820-02	0.1394540-02	-0.9477640-03
21	-0.3518910-02	0.1683010-02	-0.3018070-02	-0.8135370-02	0.5203470-02
22	-0.1969400-01	-0.5874940-02	0.3576010-03	-0.4330880-03	-0.1967470-03
23	-0.3722370-01	-0.1269020-01	-0.2153430-03	0.2385900-03	0.2674760-03
24	0.9310700-02	0.6527290-02	0.4211750-04	-0.5381380-04	0.1129130-03
25	-0.1425830-01	0.1835650-01	-0.1731860-04	0.1113100-04	-0.1902110-02
26	-0.1486180-01	0.3472910-01	-0.2303030-03	0.3313810-03	0.2991090-05
27	0.7229320-02	0.4728260-03	-0.6955880-04	0.2277040-03	-0.1036760-02
28	0.1967720+00	0.1203210+00	0.1891230-04	0.2196130-04	0.2571830-04
29	-0.2878180+00	-0.1297600+00	0.1262020-03	0.9823650-04	0.1744260-03
30	-0.1603980+00	-0.1033240+00	0.7494090-04	0.1073740-03	-0.7319990-05

	16	17	18	19	20
16	0.1207830+00				
17	-0.1154330+00	0.2412620+00			
18	-0.4711730-01	0.7605660-01	0.9497700-01		
19	0.8736350-02	0.1676400-01	-0.5868840-02	0.1074740+00	
20	-0.1311850-01	-0.2136340-01	0.8241970-02	0.1078410+00	0.2648910+00
21	-0.4618080-02	-0.8599280-02	0.6574930-02	-0.4495930-01	-0.8433450-01
22	0.6683330-03	-0.1074080-02	-0.1769610-02	0.1107280-03	0.6409820-04
23	0.7879310-03	-0.3016080-03	0.1066230-02	0.1538180-03	-0.2148820-03
24	0.1046950-02	-0.8744710-03	0.8192990-03	0.9672270-04	-0.1838240-03
25	0.1061710-03	-0.3661710-03	-0.2629230-03	-0.1025870-03	0.1378450-03
26	-0.1152800-03	0.2972970-03	0.6788340-03	-0.1838610-03	0.2529260-04
27	0.3220560-04	0.2676950-04	0.3405500-03	0.1229480-03	-0.2242650-04
28	-0.5561130-04	0.2306170-03	0.3620670-03	0.8816890-04	-0.1863290-03
29	-0.8231580-05	0.1110710-04	0.3994980-03	-0.1803860-03	-0.1550510-03
30	0.3196000-04	0.4219420-03	-0.1682920-04	-0.4547990-05	-0.2534740-03

	21	22	23	24	25
21	0.9766060-01				
22	-0.7311640-03	0.1503710+00			
23	-0.1109190-03	-0.1105010+00	0.2208490+00		
24	-0.2594710-03	-0.6042960-01	0.8272210-01	0.1035120+00	
25	-0.6968820-03	0.1208960-02	-0.1783290-02	0.1710870-01	0.7118910-01
26	-0.4329140-03	0.2885600-02	0.5646420-02	-0.2347300-01	0.7572320-02
27	-0.2530950-04	0.1231460-02	0.1727580-02	-0.9510790-02	-0.3268650-01
28	-0.1533570-03	-0.6614910-04	-0.3422500-02	0.5881080-03	-0.7943420-03
29	-0.6506060-04	-0.4724690-02	-0.5263400-02	0.2970340-02	0.9895430-03
30	-0.7449450-03	0.1104250-02	0.1793590-02	0.1949690-02	-0.7496320-03

	26	27	28	29	30
26	0.6529580-01				
27	-0.3200620-01	0.3405460+00			
28	-0.4296290-03	0.3219930-03	0.1485410+00		
29	0.2668420-02	0.1413100-04	-0.1679440+00	0.3244500+00	
30	0.1456440-02	0.5994350-03	-0.1136390+00	0.1460250+00	0.9870630-01

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.3570530+00				
2	0.8506380-02	0.3680290+00			
3	-0.3370240-02	0.4636500-01	0.3615410+00		
4	0.8772900-02	-0.1357790-02	-0.3131310-04	0.3644760+00	
5	0.1523980-01	-0.1211980-02	0.6266010-03	0.1693860-02	0.3433680+00
6	0.1246940-01	-0.5063150-02	0.1963860-02	0.1822970-02	0.2586720-02
7	0.2260290-03	0.1470240-01	0.1118410-01	-0.2101310-03	0.4598970-03
8	-0.1681040-02	0.1145260-01	0.1352660-01	0.2494610-03	-0.1081810-03
9	0.8290440-03	-0.1195890-02	-0.1056430-02	-0.1492580-03	-0.7496770-04
10	0.5718120-01	0.5785960-01	0.4257210-03	0.5282350-02	-0.2106940-02
11	-0.6742790-02	0.6138900-01	-0.1301740-01	0.4109670-03	0.8450540-03
12	0.5851520-01	0.4229150-02	0.2663600-02	-0.5873730-02	-0.5258700-02
13	0.5615150-01	-0.1508370-01	0.9537420-03	-0.4877580-02	-0.9269570-02

Table 7c. Force Constant Matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] at the 6-31G* MP2 Level of Calculation. (CONTINUED 2)

14	0.5812390-01	-0.8702140-02	0.7235710-02	-0.5462330-02	-0.7153980-02
15	-0.134627D-01	0.5918940-01	-0.3295270-01	-0.4399430-03	0.4127830-02
16	0.7481520-02	0.6561010-01	-0.3362510-01	0.1236770-02	0.8252460-03
17	0.2140090-02	-0.1444040-02	0.4900940-01	-0.1941000-03	-0.4128850-03
18	0.7912210-04	0.8651930-03	0.5596830-02	0.1883390-03	0.5633940-04
19	0.1982170-03	-0.1854780-02	0.1397020-02	-0.1220230-03	0.1618420-01
20	0.1252910-02	-0.3098060-02	-0.3616710-03	-0.1516600-01	0.1756870-02
21	-0.1320270-02	0.1273630-02	-0.1480260-02	0.1576370-01	-0.1879840-01
22	0.1837960-02	0.1260360-03	-0.5275210-01	0.8402520-04	0.2950400-04
23	-0.1215490-03	0.2659360-02	0.4764510-01	-0.4365540-03	0.1132090-02
24	0.3466640-02	0.9123590-03	-0.1435080-02	-0.1011670-03	-0.7526280-03
	6	7	8	9	10
6	0.3550510+00				
7	0.2621040-03	0.3450120+00			
8	-0.1032950-04	0.2713820-02	0.3481720+00		
9	-0.8073240-04	-0.1639430-02	-0.3726530-03	0.5083550+00	
10	-0.8158740-02	-0.3297050-02	0.5201370-02	0.8192950-03	0.2965960+00
11	-0.4002950-02	-0.6041400-02	-0.1930300-02	-0.8854150-02	0.1095160-01
12	-0.5148460-02	0.8780700-03	0.1546140-02	-0.1577470-03	0.2217390-01
13	-0.6337490-02	0.4249350-02	-0.5349700-03	-0.1862560-03	-0.5905670-02
14	-0.1121780-01	0.2775730-03	-0.2474340-03	0.6884970-03	0.1171520-02
15	0.5297440-03	-0.6028930-02	-0.7835930-02	-0.2688740-02	-0.3462720-02
16	0.6858120-03	-0.8091740-02	0.1221740-02	0.1948720-02	0.2667620-01
17	-0.3297710-03	0.3983330-02	-0.2545600-03	0.2120590-01	0.5385690-03
18	-0.4354320-02	0.1430860-01	-0.6520360-02	0.1519060-01	0.1144790-01
19	-0.1556480-01	-0.8111360-03	0.3588260-03	0.2015520-03	-0.1478960-02
20	0.1663370-01	0.1055040-02	-0.8855000-04	-0.1259130-03	0.3959380-02
21	-0.7063580-04	-0.3865590-03	0.3058430-03	-0.2011660-03	-0.1173210-02
22	0.1523770-03	0.1799660-02	0.1375790-01	-0.7434710-02	-0.5183880-02
23	-0.1781890-03	-0.1383180-01	-0.8152330-02	-0.5558490-02	-0.3906850-02
24	0.6849790-04	-0.1104200-03	0.1255770-02	0.3275790-02	0.2957420-02
	11	12	13	14	15
11	0.4313330+00				
12	-0.2978160-02	0.2649880+00			
13	0.2422570-02	0.2967600-01	0.2704260+00		
14	0.6156500-03	0.3136290-01	0.4146590-01	0.2658650+00	
15	0.7334630-01	0.3217460-03	-0.4224930-03	0.3000860-02	0.2844530+00
16	0.6162220-01	0.8210590-02	0.2434350-03	0.2700300-02	0.3876160-01
17	-0.3069200-01	-0.4073250-03	-0.1762350-02	-0.1654290-03	-0.1385590-01
18	-0.2609980-02	-0.4912960-02	-0.2088610-02	0.6306450-02	-0.6055570-01
19	-0.4081750-02	0.1593550-02	-0.4757000-01	0.4763460-01	-0.1263980-02
20	0.1829270-02	0.4928000-01	-0.3426780-02	-0.4977540-01	-0.1606260-02
21	0.8578330-03	-0.5094230-01	0.5304190-01	0.7022760-02	0.8638710-03
22	0.6777890-01	-0.1287880-03	0.2089930-02	0.2842690-03	0.1828670-01
23	-0.5206730-01	0.1373720-03	0.2339620-02	-0.1616710-02	0.4155890-01
24	-0.4776830-02	0.1069500-03	0.7672580-04	0.2691660-02	0.7670650-02
	16	17	18	19	20
16	0.2892160+00				
17	0.1464030-02	0.1914350+00			
18	0.5630480-01	0.2638400-01	0.3079140+00		
19	0.2161020-03	0.1410580-03	-0.1448050-02	0.1998780+00	
20	0.3716490-03	0.1248120-03	-0.4307320-02	-0.9862700-01	0.1913650+00
21	-0.5718660-03	0.5496220-04	0.1177040-02	-0.9715020-01	-0.9179580-01
22	-0.4557540-01	-0.2166000-01	-0.1387580+00	0.2131350-03	0.3350910-04
23	-0.1443270-01	-0.3364760-02	-0.1473680+00	-0.1448590-02	0.2582440-03
24	-0.3796720-02	-0.8647970-02	0.9130150-02	0.3078560-03	-0.8465520-03
	21	22	23	24	
21	0.1948020+00				
22	0.1378600-03	0.2362250+00			
23	0.5807210-03	-0.8918480-01	0.2449000+00		
24	0.6435420-03	-0.1997550-02	-0.2966790-02	0.2102000-01	

Table 7d. Force Constant Scaling Constants, Q(I), and C matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation.

Q Values

I	Q(I)
1	0.853126E+00
2	0.843029E+00
3	0.845156E+00
4	0.945018E+00
5	0.936652E+00
6	0.939081E+00
7	0.919893E+00
8	0.924169E+00
9	0.844771E+00
10	0.993949E+00
11	0.875442E+00
12	0.888762E+00
13	0.886238E+00
14	0.882170E+00
15	0.875850E+00
16	0.883703E+00
17	0.940571E+00
18	0.897695E+00
19	0.918829E+00
20	0.912346E+00
21	0.918511E+00
22	0.900908E+00
23	0.894679E+00
24	0.109520E+01

C Matrix (24,24)

	COLUMN 1	COLUMN 2	COLUMN 3
ROW 1	0.1000000000000D+01		
ROW 2	0.8520623202060+00	0.1000000000000D+01	
ROW 3	0.1017347741410+01	0.1091470465010+01	0.1000000000000+01
ROW 4	0.8493426689850+00	0.6844018900360+00	0.1000000000000+01
ROW 5	0.9355987631600+00	0.7991790625160+00	0.1000000000000+01
ROW 6	0.9054160255850+00	0.1128495765910+01	0.9309782497880+00
ROW 7	0.1000000000000+01	0.9389421564870+00	0.9151147994460+00
ROW 8	0.7848598310330+00	0.9072416246910+00	0.8891076525890+00
ROW 9	0.1000000000000+01	0.1000000000000+01	-0.1239764848510+01
ROW 10	0.1192208919710+01	0.1220982675160+01	0.1000000000000+01
ROW 11	0.1447399166110+01	0.1010914297940+01	0.1527351030240+01
ROW 12	0.1045784750900+01	0.2406868062400+01	0.9659129975000+00
ROW 13	0.1042328304870+01	0.1246196497500+01	0.7041214667450+00
ROW 14	0.1055629557240+01	0.1308947922010+01	0.1398665454630+01
ROW 15	0.1220757474000+01	0.1044460985940+01	0.1052545804410+01
ROW 16	0.1988804079460+01	0.1056670354540+01	0.1025115255960+01
ROW 17	0.9262336464030+00	0.9942611643390+00	0.1287176667810+01
ROW 18	0.1000000000000+01	0.1000000000000+01	0.1475742504260+01
ROW 19	0.1000000000000+01	0.1563327013750+01	0.1093234751300+01
ROW 20	0.8945449716360+00	0.1337573722300+01	0.1000000000000+01
ROW 21	0.9980847011800+00	0.1032081690850+01	0.1617035580700+01
ROW 22	0.1074583083980+01	0.1000000000000+01	0.1077361389910+01
ROW 23	0.1000000000000+01	0.1939928253990+01	0.1022183495030+01
ROW 24	0.1288821780470+01	0.5332402720940+00	0.1000000000000+01

	COLUMN 4	COLUMN 5	COLUMN 6

Table 7d. Force Constant Scaling Constants, Q(I), and C matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED 1)

ROW	4	0.1000000000000+01		
ROW	5	0.4496340258690+00	0.1000000000000+01	
ROW	6	0.4877698341610+00	0.5988362554720+00	0.1000000000000+01
ROW	7	0.1000000000000+01	0.4105461101910+00	0.1000000000000+01
ROW	8	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	9	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	10	0.1012848249630+01	0.7567757938310+00	0.1020099900390+01
ROW	11	0.1000000000000+01	0.6423857537660+00	0.9971046704810+00
ROW	12	0.1135643634930+01	0.9252342850410+00	0.9488995028530+00
ROW	13	0.9183488749540+00	0.1282271290280+01	0.9748639130210+00
ROW	14	0.9756355459430+00	0.1009463198100+01	0.1253643630650+01
ROW	15	0.1000000000000+01	0.1308986845740+01	0.1000000000000+01
ROW	16	0.8451568620030+00	0.7003030443940+00	0.6933829219780+00
ROW	17	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	18	0.1000000000000+01	0.1000000000000+01	0.1124947914390+01
ROW	19	0.1000000000000+01	0.1015137589330+01	0.1022877848830+01
ROW	20	0.1025053069910+01	0.1597248756920+01	0.1039231822560+01
ROW	21	0.1037693143960+01	0.1044460218370+01	0.1000000000000+01
ROW	22	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	23	0.1000000000000+01	0.1045734527240+01	0.1000000000000+01
ROW	24	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 7	COLUMN 8	COLUMN 9
ROW	7	0.1000000000000+01		
ROW	8	0.5868516287380+00	0.1000000000000+01	
ROW	9	0.8655928390290+00	0.1000000000000+01	0.1000000000000+01
ROW	10	0.8072514528920+00	0.9445408333760+00	0.1000000000000+01
ROW	11	0.1164924327800+01	0.8478675026200+00	0.1376146581250+01
ROW	12	0.8065850274130+00	0.9217164384200+00	0.1000000000000+01
ROW	13	0.1309921521530+01	0.1000000000000+01	0.1000000000000+01
ROW	14	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	15	0.1482732685240+01	0.1017898456950+01	0.1498389628320+01
ROW	16	0.1028751378180+01	0.1000000000000+01	0.1000000000000+01
ROW	17	0.9111123742710+00	0.1000000000000+01	0.1259079641460+01
ROW	18	0.1068303321600+01	0.7849499988980+00	0.1334482430040+01
ROW	19	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	20	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	21	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	22	0.1038127647680+01	0.1023850431080+01	0.1337467647320+01
ROW	23	0.1031401245080+01	0.1404781429120+01	0.1253048176160+01
ROW	24	0.1000000000000+01	0.1000000000000+01	0.1149312216880+01

		COLUMN 10	COLUMN 11	COLUMN 12
ROW	10	0.1000000000000+01		
ROW	11	0.1437145525660+01	0.1000000000000+01	
ROW	12	0.9852270856560+00	0.1575154174950+01	0.1000000000000+01
ROW	13	0.9565180114740+00	0.8218336049700+00	0.1003442467910+01
ROW	14	0.1000000000000+01	0.1000000000000+01	0.1007624328610+01
ROW	15	0.8171009046270+00	0.1021486239670+01	0.1000000000000+01
ROW	16	0.1079078334170+01	0.9786982580960+00	0.1106724680500+01
ROW	17	0.1000000000000+01	0.1057041711190+01	0.1000000000000+01
ROW	18	0.1267653859110+01	0.1000000000000+01	0.1287445694390+01
ROW	19	0.1000000000000+01	0.1316085911230+01	0.1306705646560+01
ROW	20	0.8748526951370+00	0.8818351418890+00	0.1013622521210+01
ROW	21	0.1008521990790+01	0.8969385526100+00	0.1017299514010+01
ROW	22	0.1276434025130+01	0.1002496772110+01	0.1000000000000+01
ROW	23	0.1743659825120+01	0.9519278724260+00	0.1000000000000+01
ROW	24	0.1174493066760+01	0.1183696740490+01	0.1000000000000+01

		COLUMN 13	COLUMN 14	COLUMN 15
ROW	13	0.1000000000000+01		
ROW	14	0.1049842189040+01	0.1000000000000+01	
ROW	15	0.1000000000000+01	0.1000468263550+01	0.1000000000000+01
ROW	16	0.1000000000000+01	0.1030141901470+01	0.1004939578690+01
ROW	17	0.1220747273190+01	0.1000000000000+01	0.1069474975010+01
ROW	18	0.1631476105640+01	0.1436850890680+01	0.9736115182850+00

Table 7d. Force Constant Scaling Constants, Q(I), and C matrix for Hydroxymethyl Methyl Ether [$C_2H_6O_2$] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED 2)

ROW	19	0.1003274236470+01	0.1009283242430+01	0.1002656382290+01
ROW	20	0.3293199014630+01	0.1013631831410+01	0.1283519218460+01
ROW	21	0.1022287175460+01	0.2118484033220+01	0.1000000000000+01
ROW	22	0.1359284246550+01	0.1000000000000+01	0.9831148421750+00
ROW	23	0.1203121730290+01	0.1385080271590+01	0.1003363253460+01
ROW	24	0.1000000000000+01	0.1204945341740+01	0.1172414664540+01

		COLUMN 16	COLUMN 17	COLUMN 18
ROW	16	0.1000000000000+01		
ROW	17	0.6309831506720+00	0.1000000000000+01	
ROW	18	0.9598611471860+00	0.9573876727190+00	0.1000000000000+01
ROW	19	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	20	0.1000000000000+01	0.1000000000000+01	0.1513143018830+01
ROW	21	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	22	0.1025175407890+01	0.1003393660920+01	0.9872129898360+00
ROW	23	0.7858188568510+00	0.7368597096140+00	0.9826486054320+00
ROW	24	0.1260535352440+01	0.1202770840500+01	0.1077654459940+01

		COLUMN 19	COLUMN 20	COLUMN 21
ROW	19	0.1000000000000+01		
ROW	20	0.1001564320670+01	0.1000000000000+01	
ROW	21	0.9986418627020+00	0.9976380262260+00	0.1000000000000+01
ROW	22	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	23	0.1284650014400+01	0.1000000000000+01	0.1000000000000+01
ROW	24	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 22	COLUMN 23	COLUMN 24
ROW	22	0.1000000000000+01		
ROW	23	0.1003811568800+01	0.1000000000000+01	
ROW	24	0.1469586807940+01	0.1012920246060+01	0.1000000000000+01

Table 8a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Ethylene Glycol [$C_2H_6O_2$] Based on Several Levels of Calculation.

H6 H8

H5 O1 C2 C3 O4 H10

H7 H9

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
geometry					
$r(O_1\text{-}C_2)$/A	1.4404	1.4702	1.4024	1.4253	-
$r(C_2\text{-}C_3)$/A	1.5209	1.5325	1.5180	1.5162	-
$r(C_3\text{-}O_4)$/A	1.4404	1.4702	1.4016	1.4245	-
$r(O_1\text{-}H_5)$/A	0.9656	0.9918	0.9467	0.9713	-
$r(C_2\text{-}H_6)$/A	1.0821	1.0958	1.0865	1.0972	-
$r(C_2\text{-}H_7)$/A	1.0821	1.0958	1.0810	1.0910	-
$r(C_3\text{-}H_8)$/A	1.0821	1.0958	1.0868	1.0974	-
$r(C_3\text{-}H_9)$/A	1.0821	1.0958	1.0901	1.1010	-
$r(O_4\text{-}H_{10})$/A	0.9656	0.9918	0.9463	0.9707	-
$\phi(C_3\text{-}C_2\text{-}O_1)$/°	110.3026	110.7887	111.3454	111.2456	-
$\phi(O_4\text{-}C_3\text{-}C_2)$/°	105.4506	104.9777	107.4278	106.6895	-
$\phi(H_5\text{-}O_1\text{-}C_2)$/°	110.9909	107.4080	109.6725	107.3550	-
$\phi(H_6\text{-}C_2\text{-}C_3)$/°	109.3948	109.0933	109.5668	109.5086	-
$\phi(H_7\text{-}C_2\text{-}C_3)$/°	109.3948	109.0933	109.4336	109.4791	-
$\phi(H_8\text{-}C_3\text{-}C_2)$/°	109.3948	109.0933	109.2262	109.0085	-
$\phi(H_9\text{-}C_3\text{-}C_2)$/°	109.3948	109.0933	109.7310	109.5718	-
$\phi(H_{10}\text{-}O_4\text{-}C_3)$/°	110.9909	107.4080	109.9565	107.9402	-
$\tau(O_4\text{-}C_3\text{-}C_2\text{-}O_1)$/°	179.4521	178.3442	180.2479	179.7933	-
$\tau(H_5\text{-}O_1\text{-}C_2\text{-}C_3)$/°	77.7369	72.0405	75.2548	72.3399	-
$\tau(H_6\text{-}C_2\text{-}C_3\text{-}O_4)$/°	-56.2601	-56.3601	-55.6891	-55.6484	-
$\tau(H_7\text{-}C_2\text{-}C_3\text{-}O_4)$/°	62.3263	62.0076	62.1977	62.5023	-
$\tau(H_8\text{-}C_3\text{-}C_2\text{-}O_1)$/°	58.3996	56.9676	58.9471	58.4230	-
$\tau(H_9\text{-}C_3\text{-}C_2\text{-}O_1)$/°	-60.3484	-61.1579	-58.9099	-59.3910	-
$\tau(H_{10}\text{-}O_4\text{-}C_3\text{-}C_2)$/°	-175.5435	-176.2787	-175.9929	-175.7818	-
E/a.u.	-227.651893	-228.073723	-228.921844	-229.552275	-

Table 8a. Optimized Geometries, Total Energies and Calculated Wavenumbers $\tilde{\nu}$ for Ethylene Glycol [$C_2H_6O_2$] Based on Several Levels of Calculation. (CONTINUED)

H6 H8

H5 O1 C2 C3 O4 H10

H7 H9

parameter	3-21G	3-21G MP2	6-31G*	6-31G* MP2	Experiment
frequencies (cm^{-1})					
$\tilde{\nu}_1$	150	141	155	149	
ν_2	280	260	275	263	
ν_3	290	286	306	291	
ν_4	297	320	327	326	
ν_5	492	460	516	487	
ν_6	905	865	879	839	
ν_7	1054	984	1093	1043	
ν_8	1122	1024	1179	1106	
ν_9	1129	1042	1198	1111	
ν_{10}	1165	1116	1204	1130	
ν_{11}	1298	1222	1326	1240	
ν_{12}	1333	1271	1353	1273	
ν_{13}	1448	1375	1432	1347	
ν_{14}	1481	1409	1503	1404	
ν_{15}	1512	1428	1530	1429	
ν_{16}	1585	1498	1624	1511	
ν_{17}	1688	1613	1666	1579	
ν_{18}	1707	1634	1684	1595	
ν_{19}	3212	3073	3167	3052	
ν_{20}	3226	3087	3212	3101	
ν_{21}	3243	3111	3226	3119	
ν_{22}	3279	3145	3301	3201	
ν_{23}	3871	3516	4111	3778	
ν_{24}	3879	3522	4122	3790	

Table 8b. Force Constant Matrix for Ethylene Glycol [$C_2H_6O_2$] at the 6-31G* HF Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.937921D-01				
2	-0.141541D+00	0.610779D+00			
3	-0.342040D-01	0.154048D+00	0.506696D+00		
4	-0.781587D-01	0.944505D-02	-0.109159D-01	0.616732D+00	
5	0.820219D-02	-0.118499D+00	0.329519D-01	-0.160516D-01	0.739058D+00
6	0.731392D-02	-0.215762D-01	-0.297555D+00	-0.402040D-01	0.922091D-02
7	0.117520D-01	0.136750D-02	0.763930D-02	-0.246074D+00	-0.911757D-05
8	0.971135D-03	0.174399D-02	-0.123365D-02	0.438765D-04	-0.104683D+00
9	-0.361968D-01	-0.228375D-07	-0.381676D-01	-0.392011D-01	-0.156831D-02
10	-0.992304D-02	-0.229672D-03	-0.119972D-01	0.114927D-01	-0.603280D-03
11	-0.582454D-03	0.257596D-02	-0.359419D-03	0.299822D-05	0.161943D-02
12	-0.842235D-02	-0.350704D-03	-0.504978D-02	0.591939D-02	-0.303689D-03
13	-0.355698D-01	0.129912D+00	0.462567D-01	-0.209958D-02	0.159596D-02
14	0.132178D+00	-0.513107D+00	-0.184038D+00	-0.959024D-04	0.264282D-02
15	0.325659D-01	-0.123748D+00	-0.106950D+00	0.138947D-01	-0.515232D-01
16	0.600450D-02	0.368941D-02	0.194583D-02	-0.137212D+00	-0.107655D+00
17	0.278473D-02	0.936990D-02	0.159373D-02	-0.109642D+00	-0.244334D+00
18	0.206075D-01	0.335363D-01	-0.361338D-01	0.458373D-01	0.649923D-01
19	0.449580D-02	-0.248747D-02	0.362759D-03	-0.129696D+00	0.113482D+00
20	-0.176494D-02	0.460265D-02	-0.365872D-02	0.116304D+00	-0.276680D+00
21	0.185571D-01	-0.424344D-01	-0.254375D-01	0.331244D-01	-0.537362D-01
22	0.338822D-02	0.246236D-02	-0.354168D-03	-0.181944D-01	-0.341480D-01
23	0.516170D-03	0.697931D-03	-0.186378D-02	0.189947D-02	0.790314D-03
24	0.108128D-02	-0.628715D-05	0.183680D-02	-0.663058D-02	-0.113922D-01
25	0.363070D-02	-0.256451D-02	0.222466D-03	-0.174218D-01	0.351696D-01
26	-0.817087D-03	0.117004D-02	0.243732D-02	-0.179935D-02	0.475491D-03
27	0.110879D-02	0.440367D-03	0.260268D-02	-0.684489D-02	0.114955D-01
28	0.588265D-03	-0.531827D-04	0.104426D-02	0.630809D-03	0.166111D-04
29	0.538197D-04	0.666632D-03	0.122047D-03	-0.106805D-03	-0.390036D-03
30	-0.241130D-02	0.902784D-04	-0.184251D-02	0.502076D-02	-0.137165D-03

	6	7	8	9	10
6	0.598639D+00				
7	-0.312713D-01	0.646496D+00			
8	0.779999D-03	0.810665D-02	0.682480D+00		
9	-0.869162D-01	-0.234532D-01	-0.384179D-02	0.595409D+00	
10	-0.444735D-01	-0.122597D+00	-0.378996D-02	-0.326555D-02	0.627283D+00
11	-0.998598D-03	-0.397553D-02	-0.788044D-01	-0.171905D-02	0.413342D-01
12	-0.309519D-01	0.433157D-01	0.420398D-02	-0.295852D+00	0.172222D+00
13	-0.208259D-03	0.200585D-02	-0.325246D-02	-0.303208D-02	-0.989639D-03
14	0.767491D-02	-0.133634D-02	0.172863D-03	0.176335D-03	0.552538D-03
15	-0.182359D-01	0.279313D-03	-0.161512D-02	-0.951837D-03	0.121390D-03
16	0.450207D-01	-0.194079D-01	-0.343395D-01	0.129445D-01	0.309312D-02
17	0.710719D-01	0.198133D-02	0.733189D-03	0.181344D-02	0.737370D-04
18	-0.902464D-01	-0.669257D-02	-0.101804D-01	0.594163D-02	0.105931D-02
19	0.375374D-01	-0.191047D-01	0.351193D-01	0.104602D-01	0.292145D-02
20	-0.659978D-01	-0.205901D-02	0.144815D-02	-0.100788D-02	0.416365D-04
21	-0.763213D-01	-0.634029D-02	0.112646D-01	0.524291D-02	0.105210D-02
22	0.129471D-01	-0.129681D+00	-0.105216D+00	0.370166D-01	0.444500D-02
23	0.145534D-02	-0.109145D+00	-0.255487D+00	0.646788D-01	0.314005D-02
24	0.523668D-02	0.353584D-01	0.613114D-01	-0.840737D-01	0.225536D-01
25	0.130588D-01	-0.130403D+00	0.101905D+00	0.349394D-01	0.498310D-02
26	-0.195214D-02	0.104031D+00	-0.247092D+00	-0.595375D-01	-0.258969D-02
27	0.457064D-02	0.325888D-01	-0.570934D-01	-0.803505D-01	0.230344D-01
28	0.279072D-03	0.701351D-02	0.452300D-03	0.978809D-02	-0.520708D+00
29	0.321657D-03	0.103841D-02	-0.512998D-03	0.100608D-02	-0.379296D-01
30	-0.821969D-02	-0.514241D-01	-0.359554D-02	-0.202822D-01	-0.160307D+00

	11	12	13	14	15
11	0.575073D-01				
12	0.139391D-01	0.529879D+00			
13	0.637291D-03	0.949084D-03	0.372894D-01		
14	-0.755819D-04	0.881412D-03	-0.130219D+00	0.505972D+00	
15	0.852241D-03	0.131508D-02	-0.456555D-01	0.172965D+00	0.130583D+00

Table 8b. Force Constant Matrix for Ethylene Glycol [$C_2H_6O_2$] at the 6-31G* HF Level of Calculation. (CONTINUED 1)

16	0.1781670-02	0.1101000-03	-0.1560940-04	-0.3293650-03	0.9933160-03
17	0.5030200-03	-0.1347690-02	0.5809400-03	0.1919360-02	0.8529100-03
18	0.5661390-04	0.1818210-02	-0.2159510-03	0.1741080-02	0.2716550-02
19	-0.1879140-02	0.3316020-03	0.3816260-03	-0.6973900-03	-0.8382680-03
20	0.5349290-03	0.1332690-02	-0.3165500-03	0.2728820-02	0.1170140-02
21	-0.2579180-03	0.1456520-02	0.2329510-02	0.8977870-03	-0.8484170-02
22	0.1744410-03	0.3283140-02	-0.2412190-03	0.5659260-04	0.1441080-03
23	0.1055460-01	0.4024560-02	0.1270260-04	-0.2172660-03	0.3873790-03
24	0.3410100-01	-0.3426220-01	-0.4391440-04	-0.5062140-04	0.1501300-03
25	0.2064830-04	0.4381540-02	-0.6925270-03	-0.8217940-04	-0.1361360-02
26	0.1051370-01	-0.5948310-02	0.1050930-02	-0.1048600-03	0.5668850-03
27	-0.3395140-01	-0.3598610-01	-0.1501470-03	-0.2970690-03	-0.1393530-03
28	-0.3751420-01	-0.2220910+00	-0.6848090-04	-0.2658440-04	-0.1435730-03
29	-0.4928910-02	-0.1643140-01	-0.1523420-05	0.6958970-04	0.9157830-04
30	-0.1166260-01	-0.1323670+00	-0.2294750-03	0.4919920-04	-0.3543450-05

	16	17	18	19	20
16	0.1408580+00				
17	0.1215190+00	0.2522390+00			
18	-0.5229550-01	-0.8340040-01	0.1101380+00		
19	0.1153550-01	-0.1682620-01	-0.5850700-02	0.1343090+00	
20	0.1386770-01	-0.2358510-01	-0.7136570-02	-0.1258550+00	0.2876260+00
21	-0.6657080-02	0.1011470-01	0.6397050-02	-0.3992930-01	0.7474620-01
22	-0.7049870-02	0.1710970-03	-0.3050970-02	0.2012390-02	0.4830880-03
23	0.3522580-03	0.1810830-02	0.1502110-04	-0.4765370-03	0.1406590-02
24	-0.3172540-02	0.3396730-04	-0.1258930-02	0.8799800-03	0.4115060-03
25	0.1934730-02	-0.7987450-03	0.5168580-03	-0.7004320-02	-0.6017710-03
26	0.8294510-03	0.1297380-02	0.4191170-03	-0.1572370-03	0.1848230-02
27	0.8686210-03	-0.4442340-03	0.2459980-03	-0.3151340-02	-0.1344150-03
28	0.2593050-03	0.1562030-03	0.8473430-04	0.1494040-03	-0.9904540-04
29	0.2844870-03	0.4649080-04	-0.4296900-04	-0.2225600-03	0.7047650-04
30	0.2420360-03	-0.2883120-03	0.3816980-03	0.1975800-03	0.2748150-03

	21	22	23	24	25
21	0.9772340-01				
22	0.7519540-03	0.1333990+00			
23	-0.3793900-03	0.1188490+00	0.2666260+00		
24	0.3199530-03	-0.4603490-01	-0.7674100-01	0.1027600+00	
25	-0.2992620-02	0.1123140-01	-0.1521190-01	-0.5337650-02	0.1333280+00
26	-0.1687960-03	0.1608660-01	-0.2613980-01	-0.8125340-02	-0.1168190+00
27	-0.1165390-02	-0.4996450-02	0.7326670-02	0.7171840-02	-0.4372990-01
28	0.1042490-03	0.6909780-03	0.6387730-04	0.1346350-02	0.4132420-03
29	-0.4664470-04	0.1081180-02	-0.4253780-04	0.4575250-03	-0.1017480-02
30	0.2684860-03	0.2937040-03	0.1096430-02	0.2119120-02	0.3024160-03

	26	27	28	29	30
26	0.2584230+00				
27	0.7309390-01	0.1013950+00			
28	0.1838920-03	0.1272130-02	0.5110310+00		
29	-0.3911670-03	-0.4358650-03	0.3682010-01	0.5412460-02	
30	-0.7850730-03	0.1655510-02	0.2083150+00	0.1495800-01	0.1582910+00

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.4233790+00				
2	0.1875390-01	0.3282800+00			
3	0.4820780-02	0.1244290-01	0.4221530+00		
4	-0.2271520-02	0.4974920-03	-0.1063670-02	0.6067610+00	
5	0.1574400-01	0.5013030-02	0.2013120-02	0.5557530-03	0.3677620+00
6	0.1174980-01	0.4898970-02	0.1661580-02	-0.2176370-02	0.4243450-02
7	0.1959160-02	0.3904810-02	0.1677170-01	-0.1439230-04	-0.5427710-03
8	0.3793750-02	0.5195600-02	0.1923110-01	-0.3859140-04	0.9495480-03
9	-0.8812320-04	-0.1465760-02	-0.2883340-02	0.5079400-05	-0.1158040-03
10	0.7749240-02	0.2321040-01	0.2382760-01	-0.3025870-02	-0.4627320-02
11	0.2634470-01	0.3046590-01	0.7775250-02	-0.1917860-02	-0.4040560-02
12	0.4635550-01	0.1124670-02	-0.1801200-02	0.1547620-01	-0.4720560-04
13	-0.3202880-01	0.3215300-01	-0.3378660-02	0.1695850-02	0.2625110-02
14	-0.3617530-01	0.3327490-01	-0.3152660-02	-0.2514300-02	-0.1174880-01
15	-0.2550690-02	0.3140760-01	-0.3229790-01	-0.3213370-03	0.5908470-02
16	-0.2443850-02	0.3056570-01	-0.3392070-01	0.1001130-02	-0.1029100-02

Table 8b. Force Constant Matrix for Ethylene Glycol [$C_2H_6O_2$] at the 6-31G* HF Level of Calculation. (CONTINUED 2)

17	0.3679700-02	0.2726820-02	0.4641790-01	-0.1970020-03	0.5688880-03
18	0.4250420-02	0.7987430-03	-0.2568510-02	0.1241270-01	-0.3064110-02
19	-0.3768420-02	0.1680530-02	-0.1665830-02	0.3119810-02	0.1151290-02
20	0.4894650-01	0.3310770-02	0.1305000-02	-0.5840920-02	-0.7798630-02
21	-0.5116790-01	-0.4330440-02	-0.9457280-03	-0.6164780-02	0.1459220-01
22	-0.1724610-02	-0.3195600-02	-0.4946030-01	0.1427970-03	-0.1258740-02
23	0.1490110-02	0.9628910-03	0.5132250-01	-0.5665320-04	-0.1374450-02
24	-0.2525660-03	-0.5085460-04	-0.8021650-03	-0.1651410-03	-0.3016620-03

	6	7	8	9	10
6	0.3834260+00				
7	0.8737690-03	0.3665360+00			
8	-0.6539780-03	0.5714710-02	0.3567180+00		
9	-0.1520100-04	0.9453550-04	-0.2400780-03	0.6100740+00	
10	-0.5145690-02	-0.4341430-02	-0.1341790-02	0.1723080-02	0.4104490+00
11	-0.3202160-02	-0.5234960-02	-0.6244990-02	0.1169330-01	0.6680480-01
12	0.3496960-02	-0.6234740-03	0.2076520-02	0.2368760-03	-0.9839070-02
13	-0.1049980-01	0.5421860-02	-0.5530620-03	-0.8137700-03	0.8011410-01
14	-0.1609840-03	-0.1185320-02	0.5811720-02	-0.5542230-03	0.7141010-01
15	-0.1271270-02	0.2185100-03	-0.1460730-01	0.3268320-02	-0.1582280-01
16	0.5233660-02	-0.1370510-01	0.6313420-03	0.2494800-02	-0.1474520-01
17	0.4307220-03	0.5548270-03	0.6503520-03	0.1578760-01	0.1259230-01
18	0.4648960-02	0.3264550-02	-0.3843720-02	-0.7544350-03	0.5657580-02
19	-0.1612810-02	0.2059530-03	0.1792900-02	0.2531710-03	0.1251370-01
20	-0.1386660-01	0.1312340-02	-0.1643440-02	0.1670300-03	-0.8315060-01
21	0.5661580-02	0.1379340-02	-0.1481130-02	-0.1699050-03	0.8090900-01
22	0.1515220-02	0.8832110-02	0.1710580-01	0.3277480-02	-0.8964030-03
23	0.1131720-02	-0.1545970-01	-0.8883130-02	-0.2701350-02	-0.1901720-02
24	0.2657600-03	0.5707580-03	-0.2513540-04	0.4826670-03	-0.1508300-03

	11	12	13	14	15
11	0.4158290+00				
12	0.1065990-02	0.2033670+00			
13	-0.1702620-01	0.6614400-02	0.2814350+00		
14	-0.1617630-01	-0.1583300-01	0.4513120-01	0.2815390+00	
15	0.7614730-01	-0.1218260-03	0.3186420-01	-0.9717860-02	0.2758640+00
16	0.7969220-01	0.3327080-02	-0.9751900-02	0.3169710-01	0.5181050-01
17	0.3806700-01	-0.5122000-04	-0.1257400-02	-0.1055840-02	0.1409430-02
18	-0.9773910-03	0.3153550-01	0.8314020-01	-0.8639450-01	-0.7847560-01
19	0.3184790-02	-0.2407580-02	-0.8653410-03	0.5109620-02	0.6732850-03
20	0.1512250-03	-0.4623670-02	-0.1926570-01	0.5874690-01	-0.1452610-02
21	-0.1563900-03	-0.2261190-01	-0.5599510-01	0.1879470-01	0.3344060-03
22	0.8413790-01	-0.1103360-02	0.1584290-02	-0.1549660-03	0.1394320-01
23	-0.8392230-01	0.1116230-03	-0.6082480-03	-0.1651870-02	0.5533520-01
24	-0.1822130-02	-0.2187810-03	-0.6185950-03	0.6697100-03	0.3572220-02

	16	17	18	19	20
16	0.2806520+00				
17	0.1465610-02	0.1979790+00			
18	0.8128270-01	-0.1913720-02	0.6467440+00		
19	0.1343320-02	0.4893760-03	-0.5548260-03	0.1006690-01	
20	-0.1772530-02	0.9466680-04	-0.1560590+00	-0.2603780-02	0.2571670+00
21	0.6269420-03	0.2906400-04	-0.1549340+00	0.5827000-02	-0.9961060-01
22	-0.5725030-01	0.5614840-02	-0.1626400+00	-0.6189030-05	0.1947400-02
23	-0.1741600-01	-0.4048880-02	-0.1632770+00	-0.1541510-02	0.1770930-02
24	-0.4265610-02	-0.5396230-03	-0.2337030-02	-0.6104660-04	-0.3187690-03

	21	22	23	24
21	0.2552370+00			
22	0.1918400-02	0.2663970+00		
23	0.2112010-02	-0.9997670-01	0.2643250+00	
24	0.1948710-04	-0.1930660-03	-0.3697560-03	0.7757190-02

Table 8c. Force Constant Matrix for Ethylene Glycol [$C_2H_6O_2$] at the 6-31G* MP2 Level of Calculation.

FORCE CONSTANTS IN CARTESIAN COORDINATES (HARTREES/BOHR).

	1	2	3	4	5
1	0.9481700-01				
2	-0.1423430+00	0.5093700+00			
3	-0.3236430-01	0.1207680+00	0.417934D+00		
4	-0.6730660-01	0.8618040-02	-0.840911D-02	0.5647660+00	
5	0.8079860-02	-0.9987210-01	0.2599320-01	-0.1630240-01	0.6824960+00
6	0.9887650-02	-0.2526460-01	-0.248474D+00	-0.4167870-01	0.8439470-02
7	0.9237370-02	0.1876090-02	0.3771240-02	-0.2295120+00	-0.1671820-03
8	0.1024150-02	0.1688470-02	-0.1469860-02	-0.4839180-04	-0.9455160-01
9	-0.3157720-01	-0.5973160-03	-0.3653730-01	-0.3572340-01	-0.1106580-02
10	-0.8454250-02	-0.4723230-03	-0.1024330-01	0.9687270-02	-0.7345030-03
11	-0.4885310-03	0.2001970-02	-0.2743850-03	-0.2965460-05	0.2121450-02
12	-0.7269320-02	-0.6365210-03	-0.3835910-02	0.2410620-02	-0.5516870-03
13	-0.4354120-01	0.1310840+00	0.4394670-01	-0.2449270-02	0.2146650-02
14	0.1331400+00	-0.4276560+00	-0.1441280+00	0.9069420-03	-0.1417910-02
15	0.2761250-01	-0.8641610-01	-0.7717550-01	0.1511230-01	-0.4642570-01
16	0.5214050-02	0.3420880-02	0.1187110-02	-0.1240920+00	-0.1021620+00
17	0.2314850-02	0.8631750-02	0.3569760-03	-0.1032240+00	-0.2267100+00
18	0.1825750-01	0.2762560-01	-0.3175890-01	0.4552800-01	0.6460330-01
19	0.3398590-02	-0.2297400-02	-0.1697090-03	-0.1158590+00	0.1079630+00
20	-0.7473690-04	0.3109070-02	-0.9700430-03	0.1072460+00	-0.2613850+00
21	0.1606450-01	-0.3619420-01	-0.2264330-01	0.3147370-01	-0.5106350-01
22	0.3152710-02	0.2272010-02	0.6923160-03	-0.1832110-01	-0.3030880-01
23	0.1442450-02	0.3759730-03	0.1542900-02	0.1434680-02	0.6328020-03
24	0.7394050-03	0.4609190-04	0.1550250-02	-0.6550540-02	-0.1010400-01
25	0.3110480-02	-0.2075570-02	0.1132690-02	-0.1737740-01	0.3153960-01
26	-0.9304400-03	0.1160810-02	0.1942850-02	-0.1898600-02	0.3087230-03
27	0.7603420-03	0.6931000-03	0.2574660-02	-0.6735450-02	0.1033610-01
28	0.4877500-03	-0.1469140-03	0.6396540-03	0.1644230-03	0.6472210-04
29	0.3477460-04	0.7875630-03	0.9872640-04	-0.4729260-04	-0.5763730-03
30	-0.2247060-02	0.5647730-04	-0.1873530-02	0.4796580-02	-0.2402860-03

	6	7	8	9	10
6	0.5206910+00				
7	-0.2888530-01	0.5854350+00			
8	0.1169820-02	0.7565360-02	0.6320650+00		
9	-0.7464950-01	-0.2465360-01	-0.4816710-02	0.5172530+00	
10	-0.3823840-01	-0.1017590+00	-0.3305020-02	-0.7742390-02	0.5328760+00
11	-0.9397340-03	-0.2913510-02	-0.6872610-01	-0.3631460-02	0.3666420-01
12	-0.3001930-01	0.3955500-01	0.2203030-02	-0.2471010+00	0.1423510+00
13	-0.1230750-02	0.2456140-02	-0.3268640-02	-0.2796700-02	-0.1032170-02
14	0.9676700-02	-0.1632050-02	0.7949690-04	0.7562240-03	0.7541140-03
15	-0.2132790-01	0.5917080-03	-0.1683750-02	-0.5415410-03	0.1696410-03
16	0.4451410-01	-0.1926640-01	-0.3071480-01	0.1100630-01	0.2555520-02
17	0.6853080-01	0.2267910-02	0.5624290-03	0.1698440-02	-0.1123360-03
18	-0.8119160-01	-0.6542450-02	-0.8914660-02	0.5501930-02	0.8677000-03
19	0.3522370-01	-0.1844320-01	0.3157690-01	0.8339140-02	0.2432280-02
20	-0.6187670-01	-0.8675280-03	0.3226330-03	-0.2908950-02	-0.1288140-03
21	-0.6573420-01	-0.6056420-02	0.1022520-01	0.4939270-02	0.6798860-03
22	0.1095120-01	-0.1155780+00	-0.9987540-01	0.3719770-01	0.3530190-02
23	-0.1914780-02	-0.1020140+00	-0.2381200+00	0.6207320-01	0.2953870-02
24	0.5041000-02	0.3663700-01	0.6153930-01	-0.7590380-01	0.1853810-01
25	0.1029360-01	-0.1152880+00	0.9670330-01	0.3335930-01	0.4162610-02
26	-0.1755010-02	0.9755240-01	-0.2330610+00	-0.5558560-01	-0.2330020-02
27	0.3840260-02	0.3175110-01	-0.5473210-01	-0.7029790-01	0.1898140-01
28	-0.8638300-03	0.2977650-02	0.2747310-03	0.1216450-01	-0.4440760+00
29	0.1527410-03	0.3125400-03	-0.1311390-02	0.1050810-02	-0.3381330-01
30	-0.7993620-02	-0.4633740-01	-0.3449660-02	-0.2231560-01	-0.1253330+00

	11	12	13	14	15
11	0.4953910-01				
12	0.1513470-01	0.4393660+00			
13	0.5863470-03	0.6970320-03	0.4512780-01		
14	0.5624070-04	0.1013680-02	-0.1322030+00	0.4250620+00	
15	0.8153880-03	0.1289500-02	-0.4195690-01	0.1311900+00	0.1035200+00
16	0.1510750-02	0.6469320-03	-0.6723110-04	-0.2465700-03	0.7849590-03
17	0.2150780-03	-0.9383980-03	0.8953440-03	0.1620730-02	0.4126950-03

Table 8c. Force Constant Matrix for Ethylene Glycol [$C_2H_6O_2$] at the 6-31G* MP2 Level of Calculation. (CONTINUED 1)

18	0.2086800-03	0.1650650-02	-0.6308210-03	0.2265990-02	0.2163620-02
19	-0.1631210-02	0.9530250-03	0.4162350-03	-0.5037090-03	-0.8151240-03
20	0.5103200-03	0.2395140-02	-0.1929740-03	0.2400490-02	0.1293300-02
21	-0.3750850-03	0.1163230-02	0.2298550-02	-0.3175260-03	-0.7884320-02
22	0.6171000-04	0.2504890-02	-0.2054520-03	0.5660880-04	0.2137790-04
23	0.9705830-02	0.3566130-02	-0.5245440-04	-0.9088510-04	0.2220380-03
24	0.2891690-01	-0.3015420-01	-0.3150530-05	-0.9967090-04	0.8365910-04
25	0.2575640-03	0.3531630-02	-0.5392340-03	-0.2957260-03	-0.1371330-02
26	0.9204360-02	-0.4498460-02	0.1156820-02	-0.2194540-03	0.6129110-03
27	-0.2968640-01	-0.3149390-01	-0.4403810-04	-0.5080080-03	-0.1962480-03
28	-0.3402940-01	-0.1850850+00	-0.1510930-03	0.1459020-04	-0.1540410-03
29	-0.4384140-02	-0.1482500-01	-0.1673480-04	0.7969240-04	0.1150390-03
30	-0.1017130-01	-0.1010730+00	-0.2656790-03	0.1362160-03	0.4606840-04
	16	17	18	19	20
16	0.1299180+00				
17	0.1139400+00	0.2332920+00			
18	-0.5050190-01	-0.7931870-01	0.9928460-01		
19	0.9379840-02	-0.1599790-01	-0.4755030-02	0.1224820+00	
20	0.1320970-01	-0.2034110-01	-0.6816680-02	-0.1185240+00	0.2723270+00
21	-0.5806670-02	0.9874700-02	0.5448650-02	-0.3685030-01	0.6851460-01
22	-0.6096120-02	0.6683960-04	-0.2725730-02	0.1957570-02	0.1333400-03
23	0.8725550-04	0.1425220-02	0.1509370-03	-0.2944350-03	0.1454920-02
24	-0.2827580-02	0.7809720-04	-0.1474320-02	0.7582790-03	0.3194180-03
25	0.2043430-02	-0.4203050-03	0.3842840-03	-0.6051010-02	-0.6899850-03
26	0.4019200-03	0.1016890-02	0.3718620-03	-0.8983970-04	0.1776210-02
27	0.7196540-03	-0.4503270-03	0.1737360-04	-0.2917160-02	-0.2164520-03
28	0.3981590-03	0.2487440-03	0.1202850-03	0.2465650-03	-0.8133070-04
29	0.3688960-03	0.7593790-04	-0.4698220-04	-0.2974610-03	0.1323670-03
30	0.2871210-03	-0.2311340-03	0.3400230-03	0.2531920-03	0.2454480-03
	21	22	23	24	25
21	0.8581110-01				
22	0.6186900-03	0.1221550+00			
23	-0.2699660-03	0.1111310+00	0.2471010+00		
24	0.2576310-04	-0.4500620-01	-0.7349520-01	0.9287730-01	
25	-0.2586230-02	0.8963720-02	-0.1477210-01	-0.4346270-02	0.1208070+00
26	-0.2893970-03	0.1522050-01	-0.2279730-01	-0.7663810-02	-0.1093700+00
27	-0.1345960-02	-0.4173050-02	0.7335050-02	0.6208710-02	-0.4033580-01
28	0.1672570-03	0.4334440-03	0.7020080-04	0.2060070-02	0.1614220-03
29	-0.4631520-04	0.1161030-02	0.2396920-03	0.3641840-03	-0.1144260-02
30	0.2109520-03	-0.7834090-04	0.8015550-03	0.1751230-02	-0.4718120-04
	26	27	28	29	30
26	0.2429270+00				
27	0.6738260-01	0.8927090-01			
28	0.2960750-03	0.1986610-02	0.4393750+00		
29	-0.1040410-03	-0.2503740-03	0.3344340-01	0.5072300-02	
30	-0.5324160-03	0.1426780-02	0.1689520+00	0.1338260-01	0.1294360+00

FORCE CONSTANTS IN INTERNAL COORDINATES (ATOMIC UNITS).

	1	2	3	4	5
1	0.3676260+00				
2	0.1790900-01	0.3119080+00			
3	0.3342230-02	0.1314250-01	0.3647510+00		
4	-0.4460870-02	0.5288250-03	-0.1232830-02	0.5126590+00	
5	0.1273850-01	0.4306810-02	0.1276990-02	-0.3669370-04	0.3428950+00
6	0.7849820-02	0.4688810-02	0.2129440-02	-0.1650820-02	0.1978150-02
7	-0.1196200-02	0.3341180-02	0.1460960-01	-0.7792790-04	-0.1942130-03
8	0.2980680-02	0.4452390-02	0.1577020-01	-0.1969930-03	0.4208050-03
9	0.2070100-03	-0.6881950-03	-0.5089060-02	-0.1000230-03	-0.2776040-03
10	0.8373580-02	0.2056270-01	0.2033120-01	-0.4024070-02	-0.3844130-02
11	0.2330410-01	0.3070230-01	0.9645780-02	-0.2733810-02	-0.3547320-02
12	0.5326550-01	0.5528900-03	-0.1856890-02	0.1812080-01	-0.1705460-03
13	-0.2891150-01	0.3257010-01	-0.3898970-02	0.2389950-02	0.3760620-02
14	-0.3195650-01	0.3267740-01	-0.4584050-02	-0.3091060-02	-0.1132130-01
15	-0.1892740-02	0.3203290-01	-0.2984970-01	-0.1327380-03	0.4868060-02
16	-0.3583040-02	0.3164310-01	-0.3062860-01	0.1626160-02	-0.1471040-02
17	0.3376680-02	0.1895900-02	0.5311960-01	-0.3520200-03	0.5292850-03
18	0.6347520-02	-0.8003380-05	-0.4079360-02	0.1352810-01	-0.9530100-03

Table 8c. Force Constant Matrix for Ethylene Glycol [$C_2H_6O_2$] at the 6-31G* MP2 Level of Calculation. (CONTINUED 2)

19	-0.357084D-02	0.933657D-03	-0.145505D-02	0.318190D-02	0.164905D-02
20	0.446765D-01	0.341572D-02	0.114662D-02	-0.580000D-02	-0.994316D-02
21	-0.488102D-01	-0.345266D-02	0.882274D-03	-0.714753D-02	0.138298D-01
22	-0.390451D-02	-0.282784D-02	-0.434851D-01	0.173157D-03	-0.106949D-02
23	0.132215D-02	0.679574D-03	0.470138D-01	-0.128406D-03	-0.118182D-02
24	-0.346069D-03	-0.123484D-03	-0.871167D-03	-0.189479D-03	-0.416482D-03
	6	7	8	9	10
6	0.359681D+00				
7	0.755001D-03	0.341823D+00			
8	-0.696841D-03	0.326818D-02	0.332364D+00		
9	-0.528199D-04	-0.360380D-03	-0.793980D-03	0.516001D+00	
10	-0.756358D-02	-0.385904D-02	-0.982687D-03	0.149234D-02	0.370914D+00
11	-0.312998D-02	-0.454038D-02	-0.540984D-02	0.145678D-01	0.587800D-01
12	0.240700D-02	-0.263843D-03	0.222776D-02	0.280979D-03	-0.104085D-01
13	-0.102411D-01	0.459305D-02	-0.110064D-02	-0.101552D-02	0.704743D-01
14	-0.333955D-03	-0.152092D-02	0.488025D-02	-0.762737D-03	0.626123D-01
15	-0.188806D-02	0.131970D-02	-0.142278D-01	0.323984D-02	-0.147344D-01
16	0.428798D-02	-0.135157D-01	0.190193D-02	0.257839D-02	-0.127789D-01
17	0.335934D-03	0.298146D-03	0.485234D-03	0.176226D-01	0.127090D-01
18	0.369373D-02	0.135611D-02	-0.162255D-02	-0.812009D-03	0.831790D-02
19	-0.163407D-02	0.240567D-03	0.187356D-02	0.366102D-03	0.108528D-01
20	-0.133859D-01	0.135567D-02	-0.141121D-02	0.225289D-03	-0.745629D-01
21	0.632153D-02	0.116763D-02	-0.178015D-02	-0.157878D-03	0.698929D-01
22	0.157135D-02	0.104616D-01	0.164037D-01	0.416214D-02	0.668379D-04
23	0.111364D-02	-0.148487D-01	-0.109630D-01	-0.361573D-02	-0.235556D-02
24	0.427063D-03	0.114976D-02	-0.576702D-03	0.552821D-03	-0.989572D-04
	11	12	13	14	15
11	0.369959D+00				
12	0.130248D-02	0.193363D+00			
13	-0.156773D-01	0.518134D-02	0.253561D+00		
14	-0.143452D-01	-0.145016D-01	0.402036D-01	0.252889D+00	
15	0.647488D-01	0.846529D-04	0.287776D-01	-0.833312D-02	0.246572D+00
16	0.689655D-01	0.323254D-02	-0.877859D-02	0.288513D-01	0.461791D-01
17	0.341669D-01	-0.147979D-03	-0.118199D-02	-0.980686D-03	0.143531D-04
18	-0.469089D-03	0.287025D-01	0.724684D-01	-0.752619D-01	-0.676997D-01
19	0.346688D-02	-0.243365D-02	-0.158960D-02	0.496922D-02	0.514065D-03
20	0.189683D-04	-0.291426D-02	-0.131016D-01	0.537639D-01	-0.228583D-02
21	0.367116D-03	-0.215451D-01	-0.512911D-01	0.128703D-01	0.447903D-03
22	0.750161D-01	-0.763301D-03	0.245309D-02	-0.362456D-04	0.798639D-02
23	-0.746719D-01	-0.839979D-04	-0.656971D-03	-0.263430D-02	0.503324D-01
24	-0.202833D-02	-0.312175D-03	-0.816826D-03	0.898494D-03	0.347654D-02
	16	17	18	19	20
16	0.251358D+00				
17	0.154863D-03	0.186305D+00			
18	0.708934D-01	-0.182602D-02	0.582165D+00		
19	0.106520D-02	0.458336D-03	0.847322D-03	0.112430D-01	
20	-0.189606D-02	-0.341223D-05	-0.138870D+00	-0.298088D-02	0.231560D+00
21	0.943974D-03	0.194779D-03	-0.140907D+00	0.478862D-02	-0.913024D-01
22	-0.526591D-01	0.397953D-02	-0.145978D+00	0.407699D-04	0.133949D-02
23	-0.122611D-01	-0.282653D-02	-0.146915D+00	-0.170504D-02	0.219125D-02
24	-0.427943D-02	-0.377277D-03	-0.300488D-02	-0.617800D-04	-0.380171D-03
	21	22	23	24	
21	0.232117D+00				
22	0.249500D-02	0.242078D+00			
23	0.161018D-02	-0.922103D-01	0.240504D+00		
24	0.339877D-04	-0.244891D-03	-0.325042D-03	0.763310D-02	

Table 8d. Force Constant Scaling Constants, Q(I), and C matrix for Ethylene Glycol [$C_2H_6O_2$] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation.

Q Values

I	Q(I)
1	0.868314E+00
2	0.950126E+00
3	0.864026E+00
4	0.844910E+00
5	0.932382E+00
6	0.938071E+00
7	0.932577E+00
8	0.931728E+00
9	0.845801E+00
10	0.903679E+00
11	0.889691E+00
12	0.950804E+00
13	0.900956E+00
14	0.898236E+00
15	0.893819E+00
16	0.895623E+00
17	0.941031E+00
18	0.900148E+00
19	0.111683E+01
20	0.900425E+00
21	0.909416E+00
22	0.908709E+00
23	0.909881E+00
24	0.984003E+00

C Matrix (24,24)

		COLUMN 1	COLUMN 2	COLUMN 3
ROW	1	0.1000000000000D+01		
ROW	2	0.105136153487D+01	0.1000000000000D+01	
ROW	3	0.800418178193D+00	0.116573388736D+01	0.1000000000000D+01
ROW	4	0.229276541540D+01	0.1000000000000D+01	0.135651937382D+01
ROW	5	0.899222955646D+00	0.912782260264D+00	0.706734910521D+00
ROW	6	0.740241343039D+00	0.101379312846D+01	0.142351603832D+01
ROW	7	-0.678508805617D+00	0.909006471779D+00	0.970411530934D+00
ROW	8	0.873501974474D+00	0.910798714963D+00	0.913953884500D+00
ROW	9	0.1000000000000D+01	0.523751372248D+00	0.206463817657D+01
ROW	10	0.121985063319D+01	0.956094056661D+00	0.965633535390+00
ROW	11	0.100642653676D+01	0.109609314887D+01	0.141494488070D+01
ROW	12	0.126462275353D+01	0.517224088862D+00	0.113740943045D+01
ROW	13	0.102056285939D+01	0.109485182998D+01	0.130794884951D+01
ROW	14	0.100026125787D+01	0.106302950025D+01	0.165049124464D+01
ROW	15	0.842305687135D+00	0.110673865818D+01	0.105166533491D+01
ROW	16	0.166255588930D+01	0.112225398425D+01	0.102645463360+01
ROW	17	0.101516502400D+01	0.735305244024D+00	0.126912183431D+01
ROW	18	0.168918266544D+01	0.1000000000000+01	0.180898849500+01
ROW	19	0.962231109283D+00	0.539332186882D+00	0.889186358761D+00
ROW	20	0.103227411036D+01	0.111542156073D+01	0.996143287252D+00
ROW	21	0.107347940221D+01	0.857728014238D+00	0.1000000000000+01
ROW	22	0.254874127402D+01	0.952353807418D+00	0.992219734250D+00
ROW	23	0.998229051778D+00	0.1000000000000+01	0.103314530848D+01
ROW	24	0.1000000000000D+01	0.1000000000000D+01	0.1000000000000+01

		COLUMN 4	COLUMN 5	COLUMN 6
ROW	4	0.1000000000000D+01		
ROW	5	0.1000000000000D+01	0.1000000000000+01	
ROW	6	0.852006018569D+00	0.498453754029D+00	0.1000000000000+01
ROW	7	0.1000000000000D+01	0.1000000000000+01	0.1000000000000+01
ROW	8	0.1000000000000D+01	0.1000000000000+01	0.1000000000000+01

Table 8d. Force Constant Scaling Constants, Q(I), and C matrix for Ethylene Glycol [$C_2H_6O_2$] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED 1)

ROW	9	0.1000000000000D+01	0.1000000000000D+01	0.1000000000000D+01
ROW	10	0.1521959830600+01	0.9050315636100+00	0.1596462846320+01
ROW	11	0.1644091643850+01	0.9639207403800+00	0.1059946944540+01
ROW	12	0.1306358426270+01	0.1000000000000+01	0.7288224539330+00
ROW	13	0.1615270908390+01	0.1563016136670+01	0.1060948791050+01
ROW	14	0.1411206674620+01	0.1052954719790+01	0.1000000000000+01
ROW	15	0.1000000000000+01	0.9025240521620+00	0.1621943646340+01
ROW	16	0.1867258417440+01	[illegible]5425229302D+01	0.8938553214280+00
ROW	17	0.1000000000000+0[illegible]	[illegible]0000000000+01	0.1000000000000+01
ROW	18	0.1249704553180+0[illegible]	[illegible]3332490+00	0.8646397968540+00
ROW	19	0.1049931176000+0[illegible]	[illegible]666407D+01	0.9898636687540+00
ROW	20	0.1138458315080+01	0.[illegible]07240360+01	0.1050352091390+01
ROW	21	0.1322670116060+01	0.[illegible]9242109390+01	0.1208886261070+01
ROW	22	0.1000000000000+01	0.923067[illegible]3460+00	0.1123227427040+01
ROW	23	0.1000000000000+01	0.9335432800050+00	0.1065116380230+01
ROW	24	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 7	COLUMN 3	COLUMN 9
ROW	7	0.1000000000000+01		
ROW	8	0.6135150763280+00	0.1000000000000+01	
ROW	9	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
ROW	10	0.9682712534760+00	0.7981382796210+00	0.9906539155970+00
ROW	11	0.9521750397800+00	0.9514551132310+00	0.1436166322200+01
ROW	12	0.1000000000000+01	0.1139833663600+01	0.1000000000000+01
ROW	13	0.9241843300250+00	0.1000000000000+01	0.1000000000000+01
ROW	14	0.1401952917080+01	0.9179043463980+00	0.1000000000000+01
ROW	15	0.1000000000000+01	0.1067330642700+01	0.1140094696810+01
ROW	16	0.1079074061450+01	0.1000000000000+01	0.1187449756200+01
ROW	17	0.1000000000000+01	0.1000000000000+01	0.1251173191610+01
ROW	18	0.4533895465000+00	0.4609395871860+00	0.1000000000000+01
ROW	19	0.1000000000000+01	0.1024413268720+01	0.1000000000000+01
ROW	20	0.1127307727060+01	0.9374948204210+00	0.1000000000000+01
ROW	21	0.9192027014450+00	0.1305678624690+01	0.1000000000000+01
ROW	22	0.1286709863350+01	0.1042179660320+01	0.1448539674900+01
ROW	23	0.1042685515690+01	0.1340377019440+01	0.1525769026010+01
ROW	24	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01

		COLUMN 10	COLUMN 11	COLUMN 12
ROW	10	0.1000000000000+01		
ROW	11	0.9812861728310+00	0.1000000000000+01	
ROW	12	0.1141254133980+01	0.1328476058690+01	0.1000000000000+01
ROW	13	0.9749060320210+00	0.1028448316150+01	0.8463577703850+00
ROW	14	0.9731900664700+00	0.9920028141700+00	0.9910879039320+00
ROW	15	0.1036138006130+01	0.9535263602340+00	0.1000000000000+01
ROW	16	0.9633293977100+00	0.9694688445590+00	0.1052865233870+01
ROW	17	0.1094446268330+01	0.9809255798950+00	0.1000000000000+01
ROW	18	0.1630118423780+01	0.1000000000000+01	0.9838242284150+00
ROW	19	0.8632903868880+00	0.1092057201470+01	0.9809329879800+00
ROW	20	0.9940917231640+00	0.1000000000000+01	0.6811949229190+00
ROW	21	0.9529006897690+00	0.1000000000000+01	0.1024673353420+01
ROW	22	0.1000000000000+01	0.9915875133610+00	0.7442545112680+00
ROW	23	0.1365994370580+01	0.9889352615360+00	0.1000000000000+01
ROW	24	0.1000000000000+01	0.1189715102040+01	0.1000000000000+01

		COLUMN 13	COLUMN 14	COLUMN 15
ROW	13	0.1000000000000+01		
ROW	14	0.9902404487580+00	0.1000000000000+01	
ROW	15	0.1006407784880+01	0.9570115927040+00	0.1000000000000+01
ROW	16	0.1002123344880+01	0.1014816550570+01	0.9961857069600+00
ROW	17	0.1020903836470+01	0.1010261666060+01	0.1110394178320-01
ROW	18	0.9678965808280+00	0.9688061268700+00	0.9617687218020+00
ROW	19	0.1000000000000+01	0.9709835647230+00	0.1000000000000+01
ROW	20	0.7550276303710+00	0.1017622873740+01	0.1754071288400+01
ROW	21	0.1011949486870+01	0.7576607337660+00	0.1000000000000+01
ROW	22	0.1711252623550+01	0.1000000000000+01	0.6355520086460+00
ROW	23	0.1000000000000+01	0.1764013926900+01	0.1008622550130+01

Table 8d. Force Constant Scaling Constants, Q(I), and C matrix for Ethylene Glycol [$C_2H_6O_2$] Based on Comparison of Force Constant Matrices at the 6-31G* HF and the 6-31G* MP2 Level of Calculation. (CONTINUED 2)

ROW	24	0.1000000000000+01	0.1000000000000+01	0.1037734794640+01
		COLUMN 16	COLUMN 17	COLUMN 18
ROW	16	0.1000000000000+01		
ROW	17	0.1150977709410+00	0.1000000000000+01	
ROW	18	0.9713780276080+00	0.1036734852450+01	0.1000000000000+01
ROW	19	0.7928567972200+00	0.1000000000000+01	0.1000000000000+01
ROW	20	0.1191169488940+01	0.1000000000000+01	0.9884097435710+00
ROW	21	0.1000000000000+01	0.1000000000000+01	0.1005193884190+01
ROW	22	0.1019578598580+01	0.7664433413490+00	0.9924059041970+00
ROW	23	0.7798779523810+00	0.7544403857930+00	0.9942428920390+00
ROW	24	0.1068669658120+01	0.1000000000000+01	0.1366180571000+01
		COLUMN 19	COLUMN 20	COLUMN 21
ROW	19	0.1000000000000+01		
ROW	20	0.1141623444440+01	0.1000000000000+01	
ROW	21	0.8154389529160+00	0.1012911482880+01	0.1000000000000+01
ROW	22	0.1000000000000+01	0.7604080511470+00	0.1430663592770+01
ROW	23	0.1097237320110+01	0.1367018770390+01	0.8381148615580+00
ROW	24	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01
		COLUMN 22	COLUMN 23	COLUMN 24
ROW	22	0.1000000000000+01		
ROW	23	0.1014322182690+01	0.1000000000000+01	
ROW	24	0.1000000000000+01	0.1000000000000+01	0.1000000000000+01

Table 9. Scaling Constants for the Force Constant Matrix Expressed in Terms of Specific Internal Coordinates. The Scaling Constants are Averages Determined from Calculations which are Summarized in Tables 1-8.

internal coordinate	scaling constant, Q
stretches	
C=O	0.772
C-H (H-(C=O)-R)	0.907
C-C	0.958
C-O (R-C-OH)	0.863
O-H (R-C-OH)	0.845
C-H (H-CHOH-R)	0.931
C-H (CH_3-R)	0.945
C-O (RC-O-CR)	0.853
bends	
H-C=O	0.922
O=C-C	0.904
H-C-C (H-(C=O)-R)	0.914
H-C-C (CH_3-C-R)	0.903
C-C-C	0.923
H-C-C (H-C-(C=O)-H)	0.896
C-C-O	0.901
H-O-C	0.946
C-O-C	0.984
H-C-O	0.891
H-C-C (H-CHOH-CHOH	0.902
torsions[a]	
H-C(=O)-C-H	0.932
O=C-C-C	0.916
H-C-C-H	0.869
O-C-C-H	0.905
H-O-C-C (internal part of chain)	1.093
H-C-C-C	0.921
O-C-C-C	0.910
H-O-C-C (end of chain)	0.984

[a] Scaling constants for torsions not present in reference set of molecules are taken to be 0.900.

Table 10a. *Optimized Geometry for R-Glyceraldehyde [CHO-HCOH-CH_2OH] Based on 3-21G Level of Calculation.* [The total energy = -339.746998 a.u.]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5111 A
$r(C_2\text{-}C_3)$	1.5211 A
$r(C_1\text{-}H_4)$	1.0819 A
$r(C_1\text{-}O_5)$	1.2092 A
$r(C_2\text{-}H_6)$	1.0849 A
$r(C_2\text{-}O_7)$	1.4343 A
$r(O_7\text{-}H_8)$	0.9708 A
$r(C_3\text{-}H_9)$	1.0820 A
$r(C_3\text{-}H_{10})$	1.0793 A
$r(C_3\text{-}O_{11})$	1.4339 A
$r(O_{11}\text{-}H_{12})$	0.9687 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	109.147 °
$\phi(H_4\text{-}C_1\text{-}C_2)$	116.003 °
$\phi(O_5\text{-}C_1\text{-}C_2)$	121.431 °
$\phi(H_6\text{-}C_2\text{-}C_1)$	109.584 °
$\phi(O_7\text{-}C_2\text{-}C_1)$	108.368 °
$\phi(H_8\text{-}O_7\text{-}C_2)$	108.703 °
$\phi(H_9\text{-}C_3\text{-}C_2)$	109.340 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	111.253 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	107.727 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	107.349 °
$\tau(H_4\text{-}C_1\text{-}C_2\text{-}C_3)$	54.734 °
$\tau(O_5\text{-}C_1\text{-}C_2\text{-}C_3)$	-125.994 °
$\tau(H_6\text{-}C_2\text{-}C_1\text{-}H_4)$	-67.483 °
$\tau(O_7\text{-}C_2\text{-}C_1\text{-}H_4)$	-189.894 °
$\tau(H_8\text{-}O_7\text{-}C_2\text{-}C_1)$	19.263 °
$\tau(H_9\text{-}C_3\text{-}C_2\text{-}C_1)$	-180.920 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	-60.159 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	56.971 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	55.001 °

Table 10b. Optimized Geometry for R-Glyceraldehyde [CHO-HCOH-CH_2OH] Based on 6-31G* Level of Calculation. [The total energy = -341.654076 a.u.]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5144 A
$r(C_2\text{-}C_3)$	1.5213 A
$r(C_1\text{-}H_4)$	1.0916 A
$r(C_1\text{-}O_5)$	1.1886 A
$r(C_2\text{-}H_6)$	1.0920 A
$r(C_2\text{-}O_7)$	1.3925 A
$r(O_7\text{-}H_8)$	0.9517 A
$r(C_3\text{-}H_9)$	1.0860 A
$r(C_3\text{-}H_{10})$	1.0833 A
$r(C_3\text{-}O_{11})$	1.3951 A
$r(O_{11}\text{-}H_{12})$	0.9492 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	111.051 °
$\phi(H_4\text{-}C_1\text{-}C_2)$	116.543 °
$\phi(O_5\text{-}C_1\text{-}C_2)$	121.948 °
$\phi(H_6\text{-}C_2\text{-}C_1)$	107.083 °
$\phi(O_7\text{-}C_2\text{-}C_1)$	110.194 °
$\phi(H_8\text{-}O_7\text{-}C_2)$	108.468 °
$\phi(H_9\text{-}C_3\text{-}C_2)$	108.792 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	110.505 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	110.685 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	108.014 °
$\tau(H_4\text{-}C_1\text{-}C_2\text{-}C_3)$	51.688 °
$\tau(O_5\text{-}C_1\text{-}C_2\text{-}C_3)$	-129.929 °
$\tau(H_6\text{-}C_2\text{-}C_1\text{-}H_4)$	-67.386 °
$\tau(O_7\text{-}C_2\text{-}C_1\text{-}H_4)$	171.924 °
$\tau(H_8\text{-}O_7\text{-}C_2\text{-}C_1)$	16.822 °
$\tau(H_9\text{-}C_3\text{-}C_2\text{-}C_1)$	-178.153 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	-59.690 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	58.870 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	57.669 °

Table 11a. Optimized Geometry for R-Erythrose [CHO-HCOH-HCOH-CH_2OH] Based on 3-21G Level of Calculation. [The total energy = -453.009395 a.u]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5087 A
$r(C_2\text{-}C_3)$	1.5182 A
$r(C_3\text{-}C_4)$	1.5167 A
$r(C_1\text{-}H_5)$	1.0780 A
$r(C_1\text{-}O_6)$	1.2121 A
$r(C_2\text{-}O_7)$	1.4259 A
$r(C_2\text{-}H_8)$	1.0841 A
$r(O_7\text{-}H_9)$	0.9710 A
$r(C_3\text{-}H_{10})$	1.0827 A
$r(C_3\text{-}O_{11})$	1.4343 A
$r(O_{11}\text{-}H_{12})$	0.9685 A
$r(C_4\text{-}H_{13})$	1.0787 A
$r(C_4\text{-}H_{14})$	1.0836 A
$r(C_4\text{-}O_{15})$	1.4482 A
$r(O_{15}\text{-}H_{16})$	0.9646 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	109.591 °
$\phi(C_4\text{-}C_3\text{-}C_2)$	111.826 °
$\phi(H_5\text{-}C_1\text{-}C_2)$	115.433 °
$\phi(O_6\text{-}C_1\text{-}C_2)$	121.024 °
$\phi(O_7\text{-}C_2\text{-}C_3)$	108.936 °
$\phi(H_8\text{-}C_2\text{-}C_3)$	108.077 °
$\phi(H_9\text{-}O_7\text{-}C_2)$	108.603 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	110.024 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	105.387 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	107.891 °
$\phi(H_{13}\text{-}C_4\text{-}C_3)$	110.240 °
$\phi(H_{14}\text{-}C_4\text{-}C_3)$	109.703 °
$\phi(O_{15}\text{-}C_4\text{-}C_3)$	103.456 °
$\phi(H_{16}\text{-}O_{15}\text{-}C_4)$	111.999 °
$\tau(C_4\text{-}C_3\text{-}C_2\text{-}C_1)$	179.251 °
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$	55.291 °
$\tau(O_6\text{-}C_1\text{-}C_2\text{-}C_3)$	-124.160 °
$\tau(O_7\text{-}C_2\text{-}C_3\text{-}C_4)$	58.695 °
$\tau(H_8\text{-}C_2\text{-}C_3\text{-}C_4)$	-62.548 °
$\tau(H_9\text{-}O_7\text{-}C_2\text{-}C_1)$	4.278 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	58.278 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	-61.878 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	-164.086 °
$\tau(H_{13}\text{-}C_4\text{-}C_3\text{-}C_2)$	-69.035 °
$\tau(H_{14}\text{-}C_4\text{-}C_3\text{-}C_2)$	52.019 °
$\tau(O_{15}\text{-}C_4\text{-}C_3\text{-}C_2)$	170.192 °
$\tau(H_{16}\text{-}O_{15}\text{-}C_4\text{-}C_3)$	-179.926 °

Table 11b. Optimized Geometry for R-Erythrose [CHO-HCOH-HCOH-CH_2OH] Based on 6-31G* Level of Calculation. [The total energy = -455.542427 a.u.]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5152 A
$r(C_2\text{-}C_3)$	1.5281 A
$r(C_3\text{-}C_4)$	1.5183 A
$r(C_1\text{-}H_5)$	1.0872 A
$r(C_1\text{-}O_6)$	1.1911 A
$r(C_2\text{-}O_7)$	1.3889 A
$r(C_2\text{-}H_8)$	1.0897 A
$r(O_7\text{-}H_9)$	0.9520 A
$r(C_3\text{-}H_{10})$	1.0881 A
$r(C_3\text{-}O_{11})$	1.4006 A
$r(O_{11}\text{-}H_{12})$	0.9495 A
$r(C_4\text{-}H_{13})$	1.0828 A
$r(C_4\text{-}H_{14})$	1.0874 A
$r(C_4\text{-}O_{15})$	1.4084 A
$r(O_{15}\text{-}H_{16})$	0.9465 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	110.692 °
$\phi(C_4\text{-}C_3\text{-}C_2)$	111.970 °
$\phi(H_5\text{-}C_1\text{-}C_2)$	116.881 °
$\phi(O_6\text{-}C_1\text{-}C_2)$	121.178 °
$\phi(O_7\text{-}C_2\text{-}C_3)$	110.127 °
$\phi(H_8\text{-}C_2\text{-}C_3)$	107.858 °
$\phi(H_9\text{-}O_7\text{-}C_2)$	108.253 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	108.989 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	106.660 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	108.065 °
$\phi(H_{13}\text{-}C_4\text{-}C_3)$	110.283 °
$\phi(H_{14}\text{-}C_4\text{-}C_3)$	109.561 °
$\phi(O_{15}\text{-}C_4\text{-}C_3)$	105.832 °
$\phi(H_{16}\text{-}O_{15}\text{-}C_4)$	110.200 °
$\tau(C_4\text{-}C_3\text{-}C_2\text{-}C_1)$	179.372 °
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$	55.848 °
$\tau(O_6\text{-}C_1\text{-}C_2\text{-}C_3)$	-124.658 °
$\tau(O_7\text{-}C_2\text{-}C_3\text{-}C_4)$	56.791 °
$\tau(H_8\text{-}C_2\text{-}C_3\text{-}C_4)$	-63.001 °
$\tau(H_9\text{-}O_7\text{-}C_2\text{-}C_1)$	3.821 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	59.701 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	-59.658 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	169.429 °
$\tau(H_{13}\text{-}C_4\text{-}C_3\text{-}C_2)$	-64.274 °
$\tau(H_{14}\text{-}C_4\text{-}C_3\text{-}C_2)$	55.703 °
$\tau(O_{15}\text{-}C_4\text{-}C_3\text{-}C_2)$	175.005 °
$\tau(H_{16}\text{-}O_{15}\text{-}C_4\text{-}C_3)$	-176.058 °

Table 12a. Optimized Geometry for R-Threose [CHO-HOCH-HCOH-CH_2OH] Based on 3-21G Level of Calculation. [The total energy = -453.009160 a.u.]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5153 A
$r(C_2\text{-}C_3)$	1.5212 A
$r(C_3\text{-}C_4)$	1.5194 A
$r(C_1\text{-}H_5)$	1.0842 A
$r(C_1\text{-}O_6)$	1.2072 A
$r(C_2\text{-}O_7)$	1.4291 A
$r(C_2\text{-}H_8)$	1.0827 A
$r(O_7\text{-}H_9)$	0.9715 A
$r(C_3\text{-}H_{10})$	1.0787 A
$r(C_3\text{-}O_{11})$	1.4428 A
$r(O_{11}\text{-}H_{12})$	0.9688 A
$r(C_4\text{-}H_{13})$	1.0822 A
$r(C_4\text{-}H_{14})$	1.0816 A
$r(C_4\text{-}O_{15})$	1.4472 A
$r(O_{15}\text{-}H_{16})$	0.9648 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	110.286 °
$\phi(C_4\text{-}C_3\text{-}C_2)$	112.138 °
$\phi(H_5\text{-}C_1\text{-}C_2)$	113.444 °
$\phi(O_6\text{-}C_1\text{-}C_2)$	123.315 °
$\phi(O_7\text{-}C_2\text{-}C_3)$	109.645 °
$\phi(H_8\text{-}C_2\text{-}C_3)$	110.858 °
$\phi(H_9\text{-}O_7\text{-}C_2)$	106.070 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	110.561 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	103.681 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	107.809 °
$\phi(H_{13}\text{-}C_4\text{-}C_3)$	110.950 °
$\phi(H_{14}\text{-}C_4\text{-}C_3)$	108.823 °
$\phi(O_{15}\text{-}C_4\text{-}C_3)$	104.015 °
$\phi(H_{16}\text{-}O_{15}\text{-}C_4)$	112.062 °
$\tau(C_4\text{-}C_3\text{-}C_2\text{-}C_1)$	171.258 °
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$	137.397 °
$\tau(O_6\text{-}C_1\text{-}C_2\text{-}C_3)$	-43.507 °
$\tau(O_7\text{-}C_2\text{-}C_3\text{-}C_4)$	-68.110 °
$\tau(H_8\text{-}C_2\text{-}C_3\text{-}C_4)$	50.905 °
$\tau(H_9\text{-}O_7\text{-}C_2\text{-}C_1)$	82.207 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	46.587 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	-72.793 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	-163.569 °
$\tau(H_{13}\text{-}C_4\text{-}C_3\text{-}C_2)$	-74.709 °
$\tau(H_{14}\text{-}C_4\text{-}C_3\text{-}C_2)$	46.237 °
$\tau(O_{15}\text{-}C_4\text{-}C_3\text{-}C_2)$	164.926 °
$\tau(H_{16}\text{-}O_{15}\text{-}C_4\text{-}C_3)$	-174.914 °

Table 12b. Optimized Geometry for R-Threose [CHO-HOCH-HCOH-CH_2OH] Based on 6-31G* Level of Calculation. [The total energy = -455.540754 a.u.]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5240 A
$r(C_2\text{-}C_3)$	1.5256 A
$r(C_3\text{-}C_4)$	1.5186 A
$r(C_1\text{-}H_5)$	1.0934 A
$r(C_1\text{-}O_6)$	1.1867 A
$r(C_2\text{-}O_7)$	1.3950 A
$r(C_2\text{-}H_8)$	1.0848 A
$r(O_7\text{-}H_9)$	0.9507 A
$r(C_3\text{-}H_{10})$	1.0843 A
$r(C_3\text{-}O_{11})$	1.4056 A
$r(O_{11}\text{-}H_{12})$	0.9496 A
$r(C_4\text{-}H_{13})$	1.0869 A
$r(C_4\text{-}H_{14})$	1.0848 A
$r(C_4\text{-}O_{15})$	1.4068 A
$r(O_{15}\text{-}H_{16})$	0.9466 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	110.622 °
$\phi(C_4\text{-}C_3\text{-}C_2)$	112.635 °
$\phi(H_5\text{-}C_1\text{-}C_2)$	115.096 °
$\phi(O_6\text{-}C_1\text{-}C_2)$	122.864 °
$\phi(O_7\text{-}C_2\text{-}C_3)$	111.589 °
$\phi(H_8\text{-}C_2\text{-}C_3)$	109.701 °
$\phi(H_9\text{-}O_7\text{-}C_2)$	107.914 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	109.024 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	105.462 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	108.375 °
$\phi(H_{13}\text{-}C_4\text{-}C_3)$	110.017 °
$\phi(H_{14}\text{-}C_4\text{-}C_3)$	109.914 °
$\phi(O_{15}\text{-}C_4\text{-}C_3)$	106.111 °
$\phi(H_{16}\text{-}O_{15}\text{-}C_4)$	110.310 °
$\tau(C_4\text{-}C_3\text{-}C_2\text{-}C_1)$	168.860 °
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$	125.021 °
$\tau(O_6\text{-}C_1\text{-}C_2\text{-}C_3)$	-56.401 °
$\tau(O_7\text{-}C_2\text{-}C_3\text{-}C_4)$	-67.312 °
$\tau(H_8\text{-}C_2\text{-}C_3\text{-}C_4)$	51.421 °
$\tau(H_9\text{-}O_7\text{-}C_2\text{-}C_1)$	81.735 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	47.550 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	-71.050 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	-170.704 °
$\tau(H_{13}\text{-}C_4\text{-}C_3\text{-}C_2)$	-66.346 °
$\tau(H_{14}\text{-}C_4\text{-}C_3\text{-}C_2)$	53.386 °
$\tau(O_{15}\text{-}C_4\text{-}C_3\text{-}C_2)$	173.470 °
$\tau(H_{16}\text{-}O_{15}\text{-}C_4\text{-}C_3)$	-171.864 °

Table 13. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for R-Glyceraldehyde [HCOH-CH_2OH] Based on 3-21G Level Optimized Geometry.

$\tilde{\nu}(cm^{-1})$	R (x 10^{-44} esu^2cm^2)
unscaled	unscaled
115.93	3.690
161.68	-8.577
268.28	-34.480
319.28	-3.344
378.77	-44.810
477.46	-145.200
588.63	66.630
679.62	242.900
773.10	-51.080
881.37	-31.080
974.03	-26.060
1040.73	-74.520
1124.81	90.920
1152.65	142.600
1212.43	-83.960
1324.98	-47.600
1381.32	-14.380
1443.97	-24.770
1488.91	80.270
1526.26	-15.110
1532.96	-51.690
1566.77	9.864
1677.70	-0.364
1912.09	8.139
3208.79	-13.160
3230.02	-25.930
3239.44	6.744
3292.52	-4.433
3825.42	7.236
3860.49	5.008

Table 14. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for R-Erythrose [CHO-HCOH-HCOH-CH_2OH] Based on 3-21G Level Optimized Geometry.

$\tilde{\nu}$(cm^{-1})	R (x 10^{-44} esu^2cm^2)
unscaled	unscaled
85.83	-5.629
115.46	1.057
143.93	22.040
191.65	-21.280
290.00	67.640
296.20	41.590
321.51	-79.900
368.94	-6.097
434.66	-42.440
470.06	-68.130
490.78	81.340
553.68	-17.160
599.86	113.900
814.27	-90.170
913.73	-168.200
962.45	97.590
1081.92	6.214
1112.99	-73.560
1140.64	-0.688
1171.98	35.340
1202.68	2.969
1235.45	-11.880
1320.32	58.030
1352.48	-32.070
1378.40	-8.745
1403.02	67.460
1443.14	-3.616
1497.62	-85.300
1514.22	16.030
1527.82	11.450
1571.48	5.862
1593.68	3.302
1691.82	2.148
1900.24	-2.775
3214.05	-7.337
3218.11	-7.230
3239.38	11.560
3290.12	-1.738
3299.60	-3.421
3820.15	5.150
3868.73	6.663
3899.95	0.362

Table 15. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for R-Threose [CHO-HOCH-HCOH-CH_2OH] Based on 3-21G Level Optimized Geometry.

$\tilde{\nu}$(cm^{-1})	R (x 10^{-44} esu^2cm^2)
unscaled	unscaled
94.73	-16.770
105.80	-22.110
145.40	-4.687
193.94	17.910
260.75	6.842
303.45	11.340
327.59	22.490
346.94	-0.305
483.34	-53.020
539.87	35.440
583.82	-55.420
658.42	13.690
664.90	-23.410
713.37	68.260
900.82	175.700
994.48	7.373
1060.02	-112.500
1089.67	-6.216
1141.16	88.070
1157.60	-230.000
1193.30	20.480
1206.28	-61.470
1303.19	17.940
1325.13	94.810
1376.51	-2.095
1430.34	24.550
1445.48	18.480
1498.83	-15.700
1505.19	4.708
1535.06	-125.600
1544.69	38.710
1581.47	16.060
1696.21	1.489
1919.01	-23.310
3205.47	-5.746
3222.05	7.986
3244.95	-6.428
3266.75	-0.348
3297.14	8.591
3822.53	15.600
3869.25	4.436
3899.12	1.769

Table 16. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for R-Glyceraldehyde [CHO-HCOH-CH_2OH] Based on 6-31G* Level Optimized Geometry.

$\tilde{\nu}$(cm^{-1})		R (x 10^{-44} esu^2cm^2)	
unscaled	scaled	unscaled	scaled
116.26	110.97	5.791	6.280
155.08	149.05	-11.490	-10.200
269.34	256.72	-10.680	-10.390
317.95	303.40	-9.847	-8.799
370.74	360.81	-78.600	-65.440
445.18	446.18	-92.260	-108.300
509.94	516.16	98.530	91.510
694.97	662.24	157.500	180.000
771.76	734.50	-29.300	-41.520
902.65	864.86	-5.899	-23.030
996.59	958.36	-6.015	-5.792
1042.73	993.22	-68.520	-56.910
1175.64	1130.04	167.000	183.100
1211.23	1140.17	-39.580	-37.770
1269.46	1201.74	-26.080	-43.100
1337.65	1275.05	-53.330	-44.470
1381.42	1325.21	-15.780	-21.450
1486.06	1426.70	12.110	15.670
1507.35	1450.84	49.190	34.030
1534.78	1463.13	15.820	23.310
1569.95	1501.47	-53.970	-9.378
1583.80	1522.48	-25.910	-68.250
1659.70	1590.14	-0.744	-0.860
2021.00	1794.54	0.384	-0.123
3161.39	3045.54	-29.710	-27.400
3206.96	3059.64	-12.280	-2.449
3225.60	3112.07	0.578	-12.280
3279.23	3163.95	-4.011	-3.777
4046.82	3719.99	12.850	13.500
4089.37	3759.10	5.321	5.279

Table 17. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for R-Erythrose [CHO-HCOH-HCOH-CH_2OH] Based on 6-31G* Level Optimized Geometry.

$\tilde{\nu}$(cm^{-1})		R (x 10^{-44} esu^2cm^2)	
unscaled	scaled	unscaled	scaled
79.63	75.96	-2.740	-2.089
96.50	92.48	12.910	12.240
141.56	135.23	11.980	13.220
194.10	186.38	-39.540	-40.470
277.40	274.44	44.460	41.330
303.17	289.11	8.211	10.560
331.15	319.08	-22.060	-33.050
373.63	359.42	-14.580	-10.300
411.69	414.66	-197.200	-151.000
443.27	445.83	259.100	142.600
478.24	470.12	-121.300	34.010
497.31	487.65	42.630	-35.180
610.88	580.60	83.320	86.210
826.03	782.47	-100.900	-94.870
923.26	885.68	-102.700	-105.200
980.52	942.71	67.490	40.650
1084.85	1036.60	62.170	101.200
1146.23	1095.95	-57.660	-55.720
1189.52	1131.05	5.965	-9.007
1218.96	1160.80	23.850	-36.100
1244.29	1178.47	-106.800	-28.530
1287.08	1218.44	64.820	36.030
1337.85	1283.13	-62.910	-75.820
1367.13	1310.70	124.300	122.900
1388.06	1328.57	1.242	1.784
1410.53	1353.01	44.830	57.600
1462.77	1400.32	-57.430	-45.020
1510.38	1446.40	-64.560	-88.320
1527.11	1453.18	32.870	50.740
1551.92	1487.94	-1.484	-0.398
1589.62	1524.14	15.100	25.260
1633.27	1568.72	0.507	-6.401
1671.27	1602.09	-0.437	-0.279
2008.40	1783.85	-7.609	-12.500
3183.53	2979.00	-19.460	-1.431
3197.69	3047.65	-22.680	23.060
3209.89	3075.91	36.860	-28.730
3265.66	3110.65	1.900	4.639
3282.26	3121.99	-4.266	-5.879
4037.54	3711.46	13.000	13.600
4089.55	3759.23	1.643	1.544
4124.43	3791.30	0.947	0.972

Table 18. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for R-Threose [CHO-HOCH-HCOH-CH_2OH] Based on 6-31G* Level Optimized Geometry.

$\tilde{\nu}$(cm^{-1})		R (x 10^{-44} esu^2cm^2)	
unscaled	scaled	unscaled	scaled
83.69	80.21	-25.710	-23.980
93.83	89.25	-14.3601	-14.450
130.27	124.68	-9.191	-14.940
189.76	181.81	8.502	7.249
259.82	248.73	14.510	13.760
290.56	286.85	6.450	28.830
306.30	291.86	23.920	2.276
345.56	330.32	-4.623	-11.420
464.34	471.76	-94.340	-103.500
491.67	485.46	92.360	97.310
523.54	525.84	-3.019	43.530
559.58	549.78	-76.640	-103.700
628.49	600.28	37.160	36.940
741.40	706.28	69.570	58.240
920.52	881.49	145.000	154.500
1016.38	971.22	32.760	44.970
1073.02	1028.75	-114.000	-113.900
1129.09	1072.07	-6.807	-41.280
1188.19	1135.01	-129.200	-78.760
1211.74	1145.83	19.280	-23.940
1231.09	1173.59	-37.240	-35.870
1268.26	1201.26	-155.400	-101.100
1311.98	1263.21	52.830	47.700
1346.33	1296.43	110.500	72.780
1388.35	1325.18	10.320	9.094
1430.30	1371.14	66.980	84.700
1439.19	1373.31	50.850	51.190
1516.86	1448.77	-43.060	-0.990
1536.98	1467.97	-44.130	-75.130
1555.66	1491.01	-81.050	-120.000
1568.31	1507.38	57.070	65.510
1624.07	1557.17	1.234	37.720
1673.20	1603.84	1.234	1.420
2030.24	1800.85	-35.710	-38.730
3186.84	3007.74	-3.132	-2.435
3206.55	3035.07	16.180	3.245
3246.47	3070.40	11.790	11.420
3249.91	3103.10	-38.760	-5.625
3267.69	3136.48	34.870	14.500
4067.21	3738.73	7.142	6.969
4091.08	3760.64	1.777	1.837
4123.45	3790.40	2.796	2.809